

STIC Search Report

EIC 1700

STIC Database Tracking Number: 129676

To: John Hardee
Location: 9A41
Art Unit : 1751
August 18, 2004
Case Serial Number: 10/693733

From: John Calve
Location: CP 3/4; 3D62
Phone: 308-4139

John.Calve@uspto.gov

Search Notes

Hi John,

I didn't find much art for the structures. The first 15 records (1-62 pgs) have either fragrance or aroma etc. or are records related to cosmetics. If utility is important for this compound, then the first 15 records are the only one that may be related to fragrance. The rest of the printout (records) have nothing to do with the utility listed for claim 1. If you have any questions, please feel free to call me at your convenience.

John

703-308-4139.

4/08/00
4/12/03

4
7
11/18
23

620 02/038520
53
58
62

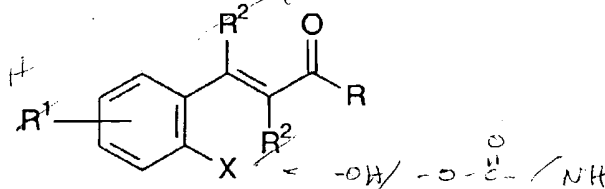
10/693,733

Good Claims

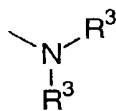
PdG

WHAT IS CLAIMED IS:

1. A photo-labile pro-fragrance conjugate having the formula:



wherein R is a unit capable of releasing a fragrance raw material having the formula:



wherein each R³ is independently hydrogen, substituted or unsubstituted C₁-C₃₀ hydrocarbyl, and mixtures thereof;

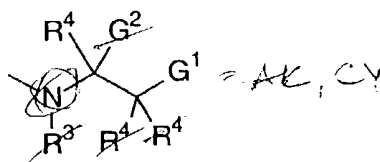
each R¹ is independently hydrogen, a unit which can substitute for hydrogen, C₁-C₁₂ substituted or unsubstituted hydrocarbyl unit;

each R² is independently hydrogen, C₁-C₁₂ substituted or unsubstituted hydrocarbyl unit, and mixtures thereof;

X is selected from the group consisting of -OH, -OC(O)R¹², -OC(O)OR¹², -NHR¹², and mixtures thereof; and

R¹² is H, C₁-C₁₂ substituted or unsubstituted alkyl, and mixtures thereof.

2. A conjugate according to Claim 1 wherein R has the formula:



wherein each R⁴ is independently selected from the group consisting of:

- hydrogen;
- C₁-C₂₂ substituted or unsubstituted, branched or unbranched alkyl;
- C₂-C₂₂ substituted or unsubstituted, branched or unbranched alkenyl;
- C₂-C₂₀ substituted or unsubstituted, branched or unbranched hydroxyalkyl;
- C₇-C₂₀ substituted or unsubstituted alkylenearyl;
- C₃-C₂₀ substituted or unsubstituted cycloalkyl;
- C₆-C₂₀ aryl;

=> FILE REG

FILE 'REGISTRY' ENTERED AT 09:59:03 ON 18 AUG 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 17 AUG 2004 HIGHEST RN 727974-89-2
DICTIONARY FILE UPDATES: 17 AUG 2004 HIGHEST RN 727974-89-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> D HIS

(FILE 'HOME' ENTERED AT 08:49:40 ON 18 AUG 2004)

FILE 'HCA' ENTERED AT 08:49:47 ON 18 AUG 2004
E US20040087453/PN

L1 1 S E3

FILE 'REGISTRY' ENTERED AT 08:50:20 ON 18 AUG 2004

FILE 'HCA' ENTERED AT 08:50:26 ON 18 AUG 2004

L2 TRA L1 1 RN : 20 TERMS

FILE 'REGISTRY' ENTERED AT 08:50:29 ON 18 AUG 2004

L3 20 SEA L2

L4 17 S L3 AND 1-10/NR

FILE 'LREGISTRY' ENTERED AT 08:51:18 ON 18 AUG 2004

L5 STR

FILE 'REGISTRY' ENTERED AT 08:58:45 ON 18 AUG 2004

L6 25 S L5

FILE 'LREGISTRY' ENTERED AT 08:59:52 ON 18 AUG 2004

L7 STR L5

FILE 'REGISTRY' ENTERED AT 09:05:39 ON 18 AUG 2004

L8 32 S L7

L9 STR L7

L10 3 S L9

L11 STR L9

L12 3 S L11

L13 1716 S L7 FULL

SAVE L13 HARDEE733/A

L14 STR L7
L15 50 S L14 SSS SAM SUB=L13

FILE 'LREGISTRY' ENTERED AT 09:11:36 ON 18 AUG 2004
L16 STR L14

FILE 'REGISTRY' ENTERED AT 09:13:50 ON 18 AUG 2004
L17 23 S L16 SSS SAM SUB=L13

FILE 'LREGISTRY' ENTERED AT 09:14:43 ON 18 AUG 2004
L18 STR L16

FILE 'REGISTRY' ENTERED AT 09:18:18 ON 18 AUG 2004
L19 20 S L18 SSS SAM SUB=L13

FILE 'LREGISTRY' ENTERED AT 09:19:10 ON 18 AUG 2004
L20 STR L18

FILE 'REGISTRY' ENTERED AT 09:21:38 ON 18 AUG 2004
L21 15 S L20 SSS SAM SUB=L13

FILE 'LREGISTRY' ENTERED AT 09:22:20 ON 18 AUG 2004
L22 SCR 1843

FILE 'REGISTRY' ENTERED AT 09:23:35 ON 18 AUG 2004
L23 12 S L20 NOT L22 SSS SAM SUB=L13

FILE 'LREGISTRY' ENTERED AT 09:24:39 ON 18 AUG 2004
L24 STR L23

FILE 'REGISTRY' ENTERED AT 09:32:16 ON 18 AUG 2004
L25 12 S L24 SSS SAM SUB=L13
L26 11 S L24 NOT L22 SSS SAM SUB=L13
L27 309 S L24 NOT L22 SSS FULL SUB=L13
SAVE L27 HARDEE733A/A

FILE 'HCA' ENTERED AT 09:35:38 ON 18 AUG 2004
L28 121 S L27
L29 425 S L13
L30 112222 S 62/SX,SC
L31 4 S L28 AND L30
L32 7 S L29 AND L30

FILE 'LCA' ENTERED AT 09:38:21 ON 18 AUG 2004
L33 1495 S FRAGANC? OR PERFUM? OR PARFUM? OR COLOGNE? OR ODOR? OR AROMA?

FILE 'HCA' ENTERED AT 09:40:42 ON 18 AUG 2004
L34 549325 S L33
L35 8 S L28 AND L34
L36 42 S L29 AND L34
L37 414782 S FRAGANC? OR PERFUM? OR PARFUM? OR COLOGNE? OR ODOR? OR AROMA#
L38 6 S L28 AND L37
L39 34 S L29 AND L37
L40 7 S L31 OR L32
L41 2 S L40 AND (L38 OR L39)

FILE 'LCA' ENTERED AT 09:44:08 ON 18 AUG 2004

FILE 'REGISTRY' ENTERED AT 09:51:52 ON 18 AUG 2004
L42 19 S L28 AND 40-100/C

L42 19 S L28 AND 40-100/C

FILE 'HCA' ENTERED AT 09:52:25 ON 18 AUG 2004

L43 30 S L42

L44 91 S L28 NOT L43

L45 90 S L44 AND 1907-2003/PY, PRY

L46 89 S L44 AND 1907-2002/PY, PRY

FILE 'REGISTRY' ENTERED AT 09:53:08 ON 18 AUG 2004

L47 290 S L27 NOT L42

L48 70 S L28 AND 30-100/C

L49 51 S L48 NOT L42

L50 36 S L28 AND 35-100/C

L51 34 S L48 NOT L50

L52 0 S L44 AND (34/SX, SC OR 9/SX, SC OR 1/SC, SX)

FILE 'HCA' ENTERED AT 09:56:28 ON 18 AUG 2004

L53 37 S L44 AND (34/SX,SC OR 9/SX,SC OR 1/SC,SX)

L54 54 S L44 NOT L53

L55 506118 S 17/SC,SX

L56 2 S L54 AND L55

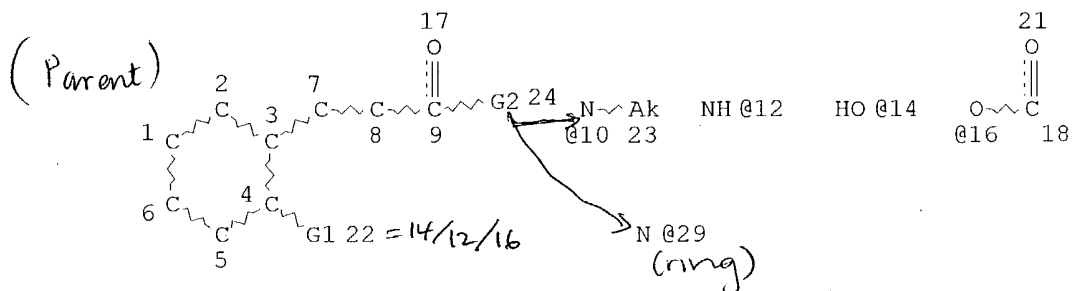
L57 15 S L31 OR L32 OR L35 OR L38 OR L40 OR L41 OR L56

L58 47 S L54 NOT L57

FILE 'REGISTRY' ENTERED AT 09:59:03 ON 18 AUG 2004

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=> D QUE STAT 127
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L7 STR



VAR G1=12/14/16

VAR G2=10/29

NODE ATTRIBUTES:

NSPEC IS R AT 29

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

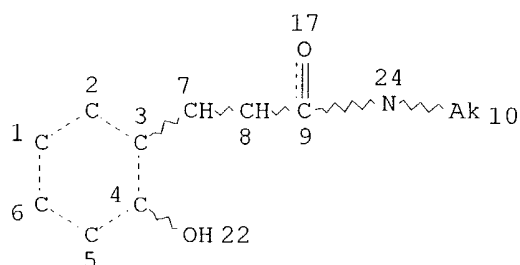
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L13 1716 SEA FILE=REGISTRY SSS FUL L7

L22 SCR 1843

L24 STR



child / Substructure

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M3 C AT 10

GRAPH ATTRIBUTES:
RSPEC 3
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L27 309 SEA FILE=REGISTRY SUB=L13 SSS FUL L24 NOT L22

100.0% PROCESSED 1294 ITERATIONS 309 ANSWERS
SEARCH TIME: 00.00.01

=> FILE HCA
FILE 'HCA' ENTERED AT 09:59:11 ON 18 AUG 2004
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FILE COVERS 1907 - 13 Aug 2004 VOL 141 ISS 8
FILE LAST UPDATED: 13 Aug 2004 (20040813/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D 157 1-15 CBIB ABS HITIND HITSTR

L57 ANSWER 1 OF 15 HCA COPYRIGHT 2004 ACS on STN
140:222903 Skin lightening compositions comprising coumarins. Harichian, Bijan; Barratt, Michael James; Bosko, Carol Annette (Unilever Home &

Personal Care Usa, Division of Conopco, Inc., USA). U.S. Pat. Appl. Publ. US 2004042983 A1 20040304, 9 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-227642 20020823.

AB Skin lightening compns. comprise coumarin derivs. and a cosmetic vehicle. Thus, a resorcinol amide was prepared by the reaction of 7-hydroxycoumarin with methylamine. A formulation contained the above amide 0.05%.,.

IC ICM A61K007-42
ICS A61K007-135

NCL 424062000

CC 62-4 (Essential Oils and Cosmetics)

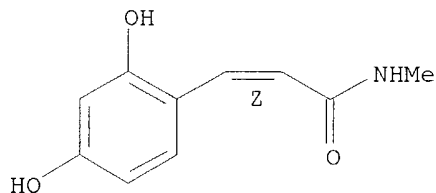
IT 664965-51-9P 664965-52-0P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(skin lightening compns. comprising coumarins)

IT 664965-51-9P 664965-52-0P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(skin lightening compns. comprising coumarins)

RN 664965-51-9 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-methyl-, (2Z)- (9CI) (CA INDEX NAME)

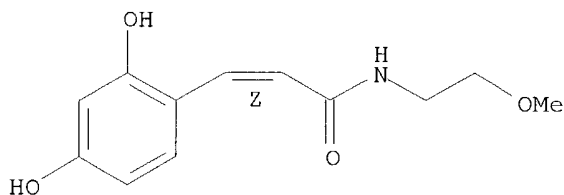
Double bond geometry as shown.



RN 664965-52-0 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-(2-methoxyethyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

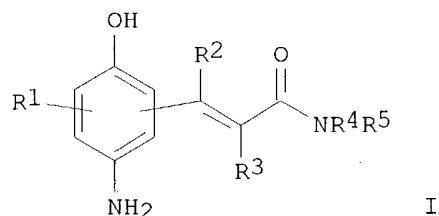


L57 ANSWER 2 OF 15 HCA COPYRIGHT 2004 ACS on STN

137:296211 (1-Amino-4-hydroxyphenyl)acrylamide derivatives and oxidative hair dyes containing them. Chassot, Laurent; Braun, Hans-Juergen (Wella Aktiengesellschaft, Germany). PCT Int. Appl. WO 2002079144 A1 20021010, 57 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (German). CODEN: PIXXD2.
APPLICATION: WO 2001-EP12126 20011019. PRIORITY: DE 2001-10115994
20010330.

GI



AB The invention relates to aminohydroxyphenylacrylamide derivs. (I; R1 = H, halogen, alkyl, hydroxyalkyl, alkoxy; R2, R3 = H, alkyl; R4, R5 = H, alkyl, unsatd. alkyl, hydroxyalkyl, alkoxy, optionally substituted aminoalkyl, cyanoalkyl, carboxyalkyl, aminocarbonylalkyl, **aromatic** group, heterocyclic group) or physiol. acceptable, water-soluble salts of I, and to oxidative hair dyes containing I as developers. I provide hair dyes with very good fastness to light and washing. Examples were given in which 3-(5-amino-2-hydroxyphenyl)acrylamide derivs. were prepared from 3-[5-(tert-butoxycarbonylamino)-2-(ethoxymethoxy)phenyl]acrylic acid and the appropriate amines or amine derivs.

IC ICM C07C237-20

ICS A61K007-13; D06P001-32; C07D295-18; C07D295-12; C07D231-38;
C07D307-52; C07D211-46; C07D207-27; C07D213-75; C07D233-61;
C07D307-22; C07D317-66; C07D207-08; C07D207-16; C07D211-42

CC 41-8 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

Section cross-reference(s): 25, 27, 28, 62

IT 467466-23-5 467466-24-6 467466-25-7 467466-26-8
467466-27-9 467466-28-0 467466-29-1 467466-30-4

RL: TEM (Technical or engineered material use); USES (Uses)

(aminohydroxyphenylacrylamide derivative developers for oxidative hair dyes)

IT 467466-33-7P 467466-34-8P 467466-35-9P 467466-36-0P

467466-37-1P 467466-38-2P 467466-39-3P 467466-40-6P

467466-41-7P 467466-42-8P 467466-43-9P

467466-44-0P 467466-45-1P 467466-46-2P

467466-47-3P 467466-48-4P 467466-49-5P

467466-50-8P 467466-51-9P 467466-52-0P

467466-53-1P 467466-54-2P 467466-55-3P

467466-56-4P 467466-57-5P 467466-58-6P

467466-59-7P 467466-60-0P 467466-61-1P 467466-62-2P 467466-63-3P

467466-64-4P 467466-65-5P 467466-66-6P 467466-67-7P

467466-68-8P 467466-69-9P 467466-70-2P

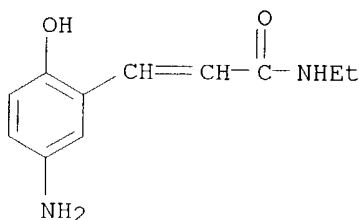
467466-71-3P 467466-72-4P 467466-73-5P

467466-74-6P 467466-75-7P 467466-76-8P

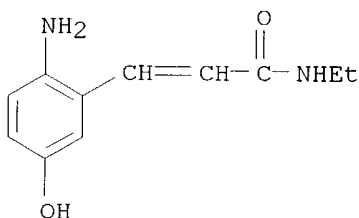
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(production of aminohydroxyphenylacrylamide derivative developers for oxidative

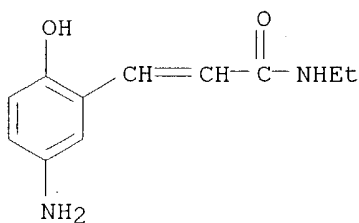
hair dyes)
IT 467466-23-5 467466-24-6
RL: TEM (Technical or engineered material use); USES (Uses)
(aminohydroxyphenylacrylamide derivative developers for oxidative hair dyes)
RN 467466-23-5 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-ethyl- (9CI) (CA INDEX NAME)



RN 467466-24-6 HCA
CN 2-Propenamide, 3-(2-amino-5-hydroxyphenyl)-N-ethyl- (9CI) (CA INDEX NAME)

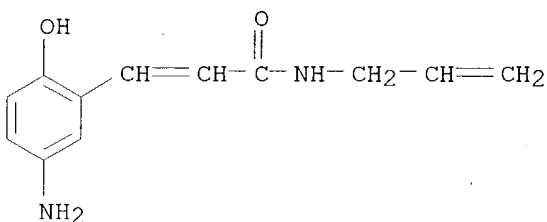


IT 467466-33-7P 467466-37-1P 467466-39-3P
467466-42-8P 467466-43-9P 467466-44-0P
467466-45-1P 467466-46-2P 467466-47-3P
467466-48-4P 467466-49-5P 467466-50-8P
467466-51-9P 467466-52-0P 467466-53-1P
467466-54-2P 467466-55-3P 467466-56-4P
467466-57-5P 467466-58-6P 467466-67-7P
467466-68-8P 467466-69-9P 467466-70-2P
467466-71-3P 467466-72-4P 467466-73-5P
467466-74-6P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(production of aminohydroxyphenylacrylamide derivative developers for oxidative hair dyes)
RN 467466-33-7 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



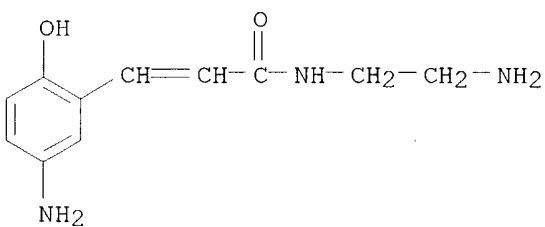
● HCl

RN 467466-37-1 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-2-propenyl-,
monohydrochloride (9CI) (CA INDEX NAME)



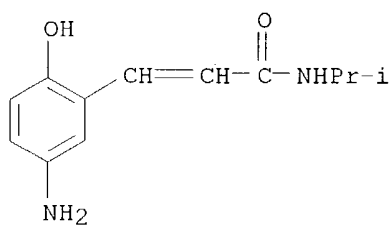
● HCl

RN 467466-39-3 HCA
CN 2-Propenamide, N-(2-aminoethyl)-3-(5-amino-2-hydroxyphenyl)-,
hydrochloride (9CI) (CA INDEX NAME)



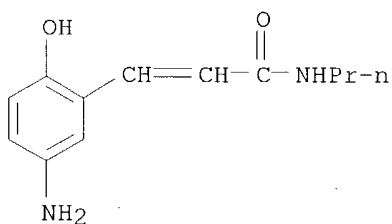
●x HCl

RN 467466-42-8 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-(1-methylethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



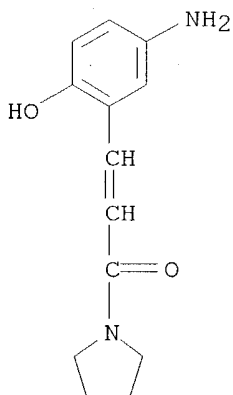
● HCl

RN 467466-43-9 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-propyl-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

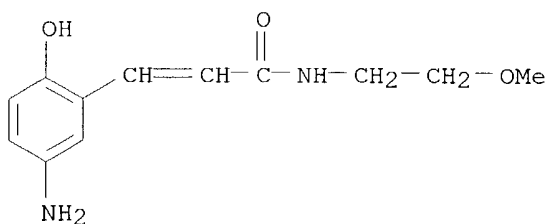
RN 467466-44-0 HCA

CN Pyrrolidine, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)

● HCl

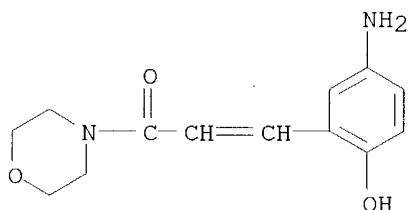
RN 467466-45-1 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-(2-methoxyethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



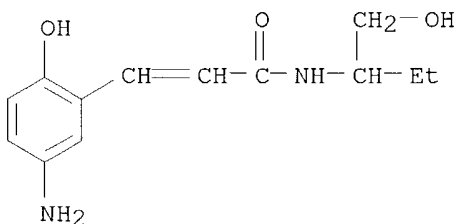
● HCl

RN 467466-46-2 HCA
CN Morpholine, 4-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



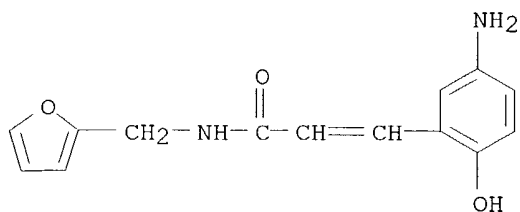
● HCl

RN 467466-47-3 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[1-(hydroxymethyl)propyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



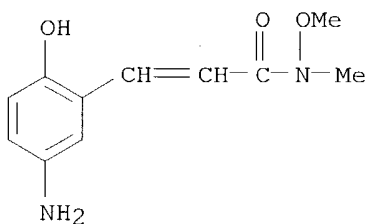
● HCl

RN 467466-48-4 HCA
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-(2-furanylmethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



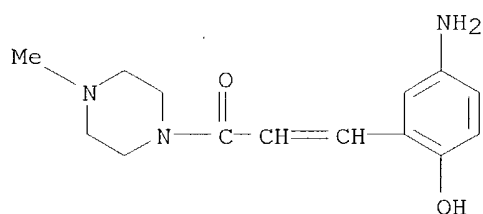
● HCl

RN 467466-49-5 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-methoxy-N-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)

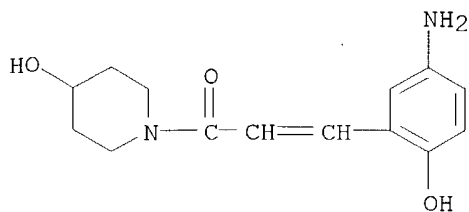
● HCl

RN 467466-50-8 HCA

CN Piperazine, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-4-methyl-,
hydrochloride (9CI) (CA INDEX NAME)●_x HCl

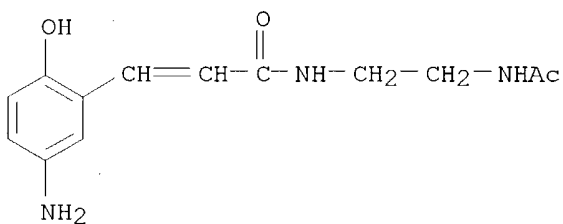
RN 467466-51-9 HCA

CN 4-Piperidinol, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



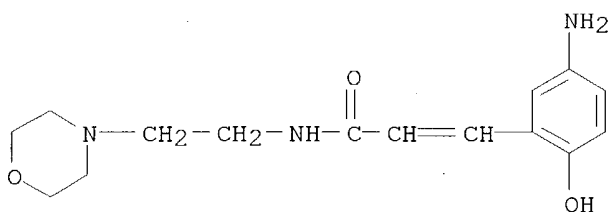
● HCl

RN 467466-52-0 HCA
 CN 2-Propenamide, N-[2-(acetylamino)ethyl]-3-(5-amino-2-hydroxyphenyl)-,
 monohydrochloride (9CI) (CA INDEX NAME)



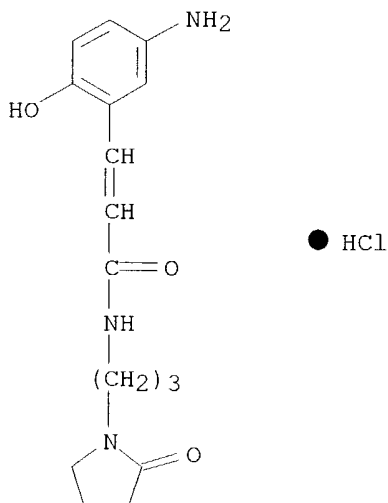
● HCl

RN 467466-53-1 HCA
 CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[2-(4-morpholinyl)ethyl]-,
 hydrochloride (9CI) (CA INDEX NAME)



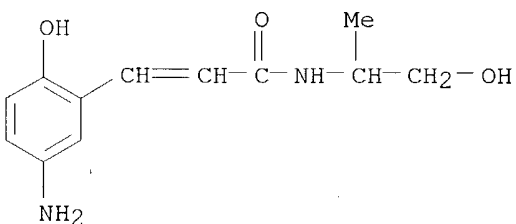
● x HCl

RN 467466-54-2 HCA
 CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[3-(2-oxo-1-pyrrolidinyl)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



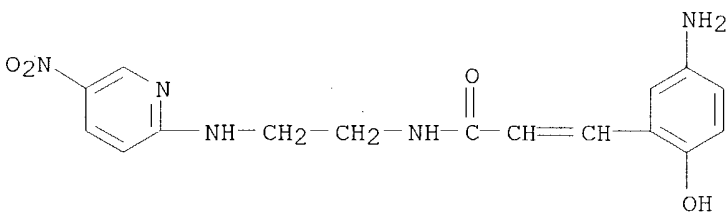
RN 467466-55-3 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-(2-hydroxy-1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



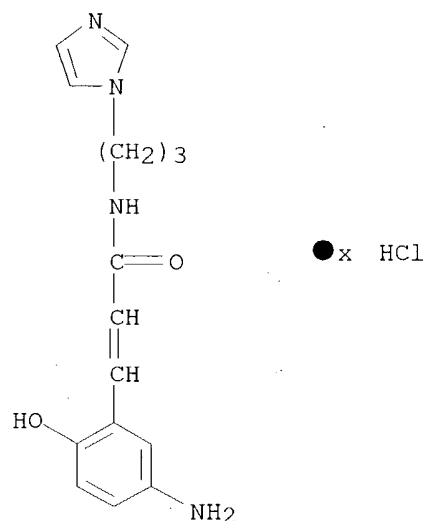
RN 467466-56-4 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[2-[(5-nitro-2-pyridinyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



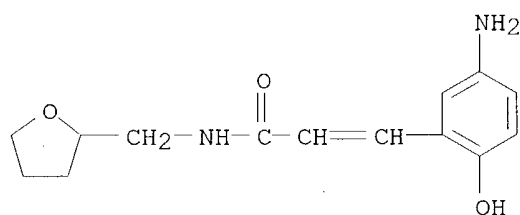
RN 467466-57-5 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[3-(1H-imidazol-1-yl)propyl]-, hydrochloride (9CI) (CA INDEX NAME)



RN 467466-58-6 HCA

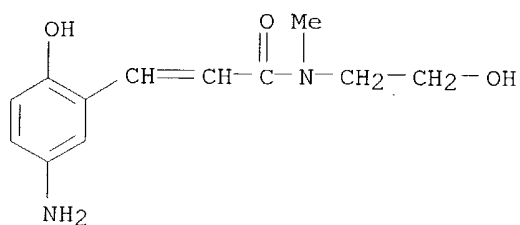
CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[(tetrahydro-2-furanyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

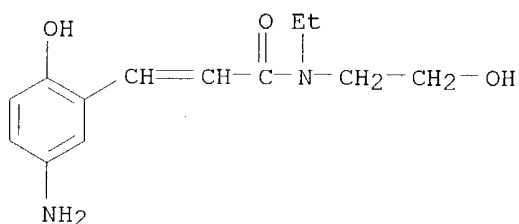
RN 467466-67-7 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-(2-hydroxyethyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



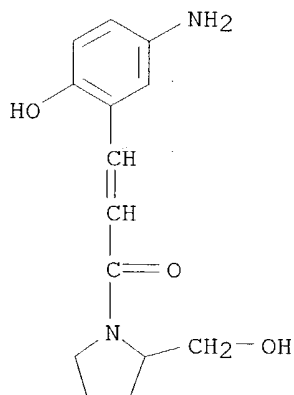
● HCl

RN 467466-68-8 HCA
 CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-ethyl-N-(2-hydroxyethyl)-,
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

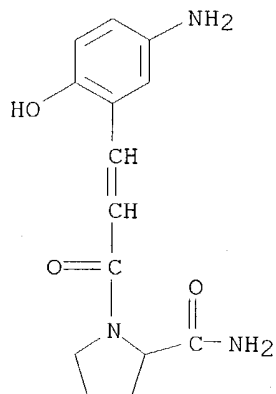
RN 467466-69-9 HCA
 CN 2-Pyrrolidinemethanol, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-,
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 467466-70-2 HCA

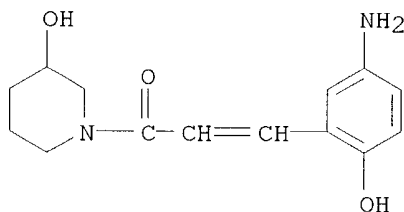
CN 2-Pyrrolidinecarboxamide, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 467466-71-3 HCA

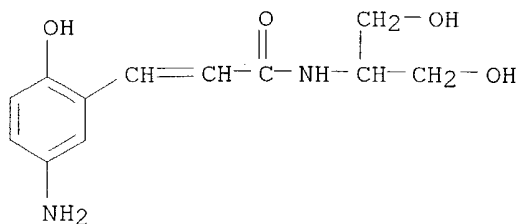
CN 3-Piperidinol, 1-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 467466-72-4 HCA

CN 2-Propenamide, 3-(5-amino-2-hydroxyphenyl)-N-[2-hydroxy-1-(hydroxymethyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



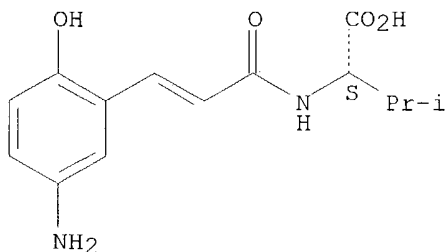
● HCl

RN 467466-73-5 HCA

CN L-Valine, N-[3-(5-amino-2-hydroxyphenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

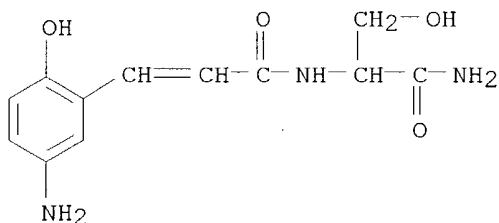
Double bond geometry unknown.



● HCl

RN 467466-74-6 HCA

CN 2-Propenamide, N-[2-amino-1-(hydroxymethyl)-2-oxoethyl]-3-(5-amino-2-hydroxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L57 ANSWER 3 OF 15 HCA COPYRIGHT 2004 ACS on STN

137:252660 Oxidative hair dyes containing 3-(2,5-diaminophenyl)-acrylamide derivatives. Chassot, Laurent; Braun, Hans-Juergen (Wella Ag, Germany). Ger. Offen. DE 10113027 A1 20020919, 20 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2001-10113027 20010317.

AB The invention concerns the synthesis of 3-(2,5-diaminophenyl)-acrylamide derivs. and their use in oxidative hair dyes as developers. Thus N-(4-aminophenyl)-3-(2,5-diaminophenyl)-acrylamide hydrochloride was synthesized and used in a hair dye composition as an 1.25 mmol ingredient with 1.25 mmol 1,3-dihydroxybenzene. Further ingredients were(g): sodium oleate 1; ascorbic acid 0.3; ethanol 1.0; ammonia (25 % aqueous solution) 1.0; water to 100.

IC ICM C07C237-20

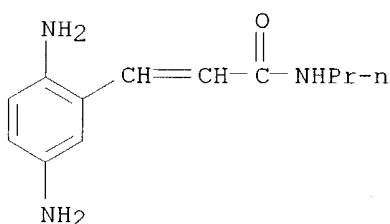
ICS C07C259-06; D06P001-32; A61K007-13; C07D295-033; C07D307-02;
C07D207-04; C07D295-16; C07D231-10; C07D401-10; C07D403-10;
C07D211-36

CC 62-3 (Essential Oils and Cosmetics)

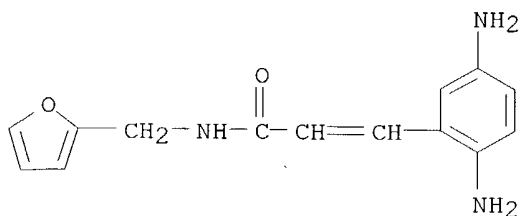
Section cross-reference(s): 25

IT 83-56-7, 1,5-Dihydroxynaphthalene 89-25-8, 3-Methyl-1-phenyl-5-pyrazolone 89-83-8, 5-Methyl-2-(1-methylethyl)phenol 90-15-3, 1-Naphthol 91-56-5, 2,3-Indolinedione 91-68-9, 3-Diethylaminophenol 92-44-4, 2,3-Dihydroxynaphthalene 95-70-5, 2,5-Diaminotoluene 95-88-5, 1-Chloro-2,4-dihydroxybenzene 99-07-0, 3-Dimethylaminophenol 106-50-3, 1,4-Diaminobenzene, biological studies 108-45-2, 1,3-Diaminobenzene, biological studies 137-19-9, 1,5-Dichloro-2,4-dihydroxybenzene 141-86-6, 2,6-Diaminopyridine 533-31-3, 3,4-Methylenedioxyphenol 575-38-2, 1,7-Dihydroxynaphthalene 582-17-2, 2,7-Dihydroxynaphthalene 591-27-5, 3-Aminophenol 608-25-3, 1,3-Dihydroxy-2-methylbenzene 619-05-6, 3,4-Diaminobenzoic acid 770-25-2, 3-[(2-Hydroxyethyl)amino]phenol 1004-74-6D, Tetraaminopyrimidine, derivs. 1687-53-2, 5-Amino-2-methoxyphenol 1953-54-4, 5-Hydroxyindole 2380-84-9, 7-Hydroxyindole 2380-86-1, 6-Hydroxyindole 2380-94-1, 4-Hydroxyindole 3131-52-0, 5,6-Dihydroxyindole 5349-76-8, 2,4-Diamino-1-methoxy-5-methylbenzene 5697-02-9, 2-Methyl-1-naphthol-acetate 6265-21-0, 3-[(2-Hydroxyethyl)amino]aniline 6941-70-4, 6-Bromo-1-hydroxy-3,4-methylenedioxybenzene 7228-00-4, 2-[(3-Hydroxyphenyl)amino]acetamide 7469-77-4, 2-Methyl-1-naphthol 7722-84-1, Hydrogen peroxide, biological studies 16461-98-6D, 1H-Pyrazole-4,5-diamine, derivs. 16867-03-1, 2-Amino-3-hydroxypyridine 26011-57-4, 6-Amino-3,4-dihydro[1,4](2H)-benzoxazine 26021-57-8, 3,4-Dihydro-6-hydroxy-1,4(2H)-benzoxazine 26455-21-0, N-(3-Dimethylaminophenyl)-urea 28020-38-4, 2,3-Diamino-6-methoxypyridine 29539-03-5, 5,6-Dihydroxyindoline 39489-79-7, 5-Amino-2,4-dichlorophenol 53222-92-7, 3-Amino-2-methylphenol 55302-96-0, 5-[(2-Hydroxyethyl)amino]-2-methylphenol 61693-42-3, 3-Amino-2,4-dichlorophenol 70643-19-5, 2,4-Diamino-1-(2-hydroxyethoxy)benzene 71077-37-7, 1,3-Diamino-4-(2-methoxyethoxy)benzene 71500-41-9, 4-Amino-2-di[(2-hydroxyethyl)amino]-1-ethoxybenzene 71500-42-0, 3-[Di(2-hydroxyethyl)amino]aniline 75513-65-4, 1,3-Diamino-4-(2,3-dihydroxypropoxy)benzene 76045-64-2, 3-[(2-Aminoethyl)amino]aniline 78661-33-3, 2-Amino-1-(2-hydroxyethoxy)-4-methylaminobenzene 80592-80-9, 3-[(2,3-Dihydroxypropyl)amino]-2-methylphenol 80592-81-0, 3-[(2-Hydroxyethyl)amino]-2-methylphenol 81892-72-0, 1,3-Di(2,4-diaminophenoxy)propane 83763-47-7, 2-Amino-4-[(2-hydroxyethyl)amino]anisole 84540-47-6, 2,6-Dihydroxy-3,4-dimethylpyridine 84540-48-7, 2,4-Diaminophenoxy acetic acid 84540-50-1, 3-Amino-2-chloro-6-methylphenol 85679-78-3, 3,5-Diamino-2,6-dimethoxypyridine 86817-42-7, 2-(4-Amino-2-hydroxyphenoxy)ethanol 90817-34-8, 3-Amino-6-methoxy-2-(methylamino)pyridine 93841-24-8, 2-(2,5-Diaminophenyl)ethanol 94082-77-6, 2,4-Diamino-1,5-di(2-hydroxyethoxy)benzene 104752-50-3, 1-(2-Aminoethoxy)-2,4-diaminobenzene 104752-51-4, 1,2-Dichloro-3,5-dihydroxy-4-methylbenzene 110102-86-8, 5-Amino-4-chloro-2-methylphenol 111451-24-2, 2,6-Diamino-3,5-dimethoxypyridine 115423-86-4, 1,3-Diamino-2,4-dimethoxybenzene 122455-85-0, 5-Amino-4-fluoro-2-methylphenol 122481-67-8, 2,4-Di[(2-hydroxyethyl)amino]-1,5-dimethoxybenzene 137290-78-9, 5-Amino-4-methoxy-2-methylphenol 137290-86-9, 5-[(2-Hydroxyethyl)amino]-4-methoxy-2-methylphenol 139443-57-5, 5-Amino-4-ethoxy-2-methylphenol 141614-04-2, 2,4-Diamino-1-ethoxy-5-methylbenzene 141614-05-3, 2,4-Diamino-1-(2-hydroxyethoxy)-5-methylbenzene 141922-20-5, 2,4-Diamino-1-fluoro-5-methylbenzene 142082-56-2, 3-[(2-Methoxyethyl)amino]phenol 146658-65-3, 5-[(3-Hydroxypropyl)amino]-2-methylphenol 149330-25-6, 2,6-Bis(2-hydroxyethyl)aminotoluene 168092-23-7, Di(2,4-

diaminophenoxy)methane 207923-07-7, 5-Amino-2-ethylphenol 244028-59-9,
5-[(2-Hydroxyethyl)amino]-1,3-benzodioxole 307493-94-3,
1,3-Diamino-4-(3-hydroxypropoxy)benzene 329320-36-7 460083-38-9
460083-39-0 460083-40-3 460083-41-4
460083-42-5 460083-43-6 460083-44-7 460083-45-8
460083-46-9 460083-47-0 460083-48-1 460083-49-2 460083-50-5
460083-51-6 460083-52-7 460084-08-6 460084-99-5
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(oxidative hair dyes containing 3-(2,5-diaminophenyl)-acrylamide derivs.)
IT 79-06-1DP, Acrylamide, 3-(2,5-diaminophenyl) derivs. 460083-53-8P
460083-54-9P 460083-55-0P 460083-56-1P
460083-57-2P 460083-58-3P 460083-59-4P 460083-60-7P
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460083-64-1P 460083-65-2P 460083-66-3P
460083-67-4P 460083-68-5P 460083-69-6P 460083-70-9P
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460083-74-3P 460083-75-4P 460083-76-5P
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460084-03-1P 460084-05-3P 460084-06-4P
460084-07-5P 460084-10-0P 460084-11-1P 460084-12-2P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation); USES (Uses)
(oxidative hair dyes containing 3-(2,5-diaminophenyl)-acrylamide derivs.)
IT 460083-38-9 460083-39-0 460083-40-3
460083-41-4 460083-43-6 460083-45-8
460083-50-5 460083-52-7
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(oxidative hair dyes containing 3-(2,5-diaminophenyl)-acrylamide derivs.)
RN 460083-38-9 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-propyl- (9CI) (CA INDEX NAME)

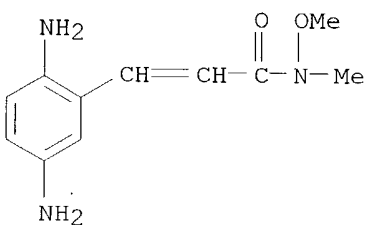


RN 460083-39-0 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(2-furanylmethyl)- (9CI) (CA INDEX NAME)



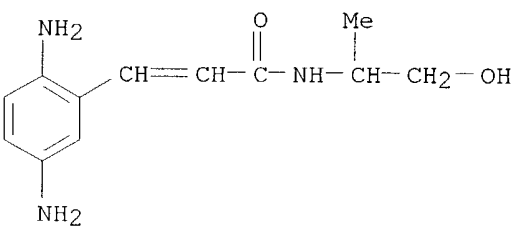
RN 460083-40-3 HCA

CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-methoxy-N-methyl- (9CI) (CA INDEX NAME)



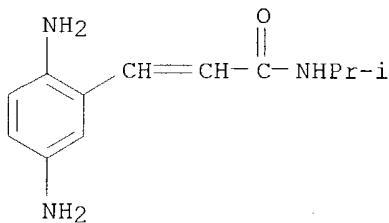
RN 460083-41-4 HCA

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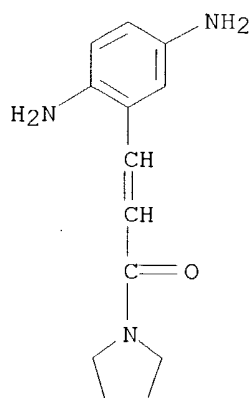
RN 460083-43-6 HCA

CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

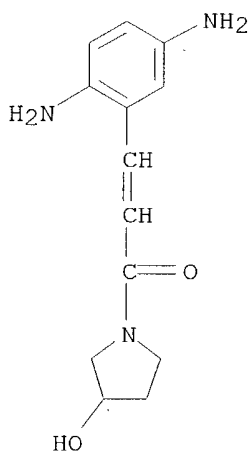


RN 460083-45-8 HCA

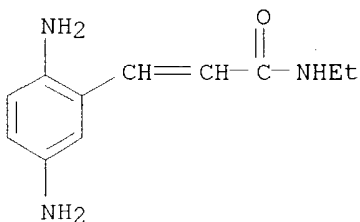
CN Pyrrolidine, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 460083-50-5 HCA
CN 3-Pyrrolidinol, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 460083-52-7 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-ethyl- (9CI) (CA INDEX NAME)



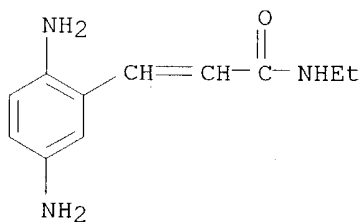
IT 460083-54-9P 460083-55-0P 460083-57-2P
460083-58-3P 460083-62-9P 460083-63-0P
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460083-67-4P 460083-69-6P 460083-72-1P
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460083-76-5P 460083-77-6P 460083-78-7P

460083-80-1P 460083-81-2P 460083-82-3P
460083-83-4P 460083-84-5P 460083-85-6P
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460084-03-1P 460084-05-3P 460084-07-5P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(oxidative hair dyes containing 3-(2,5-diaminophenyl)-acrylamide derivs.)

RN 460083-54-9 HCA

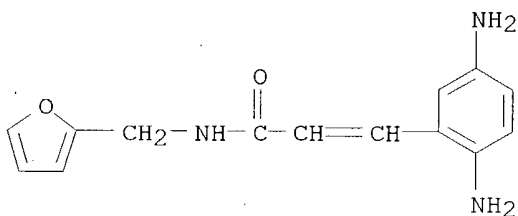
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-ethyl-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

RN 460083-55-0 HCA

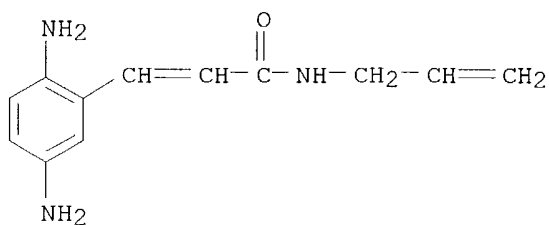
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(2-furanylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460083-57-2 HCA

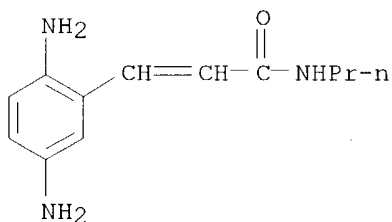
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-2-propenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460083-58-3 HCA

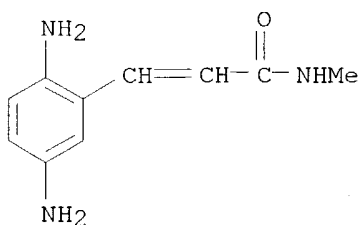
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-propyl-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

RN 460083-62-9 HCA

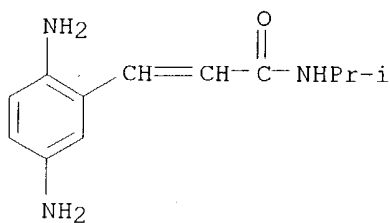
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-methyl-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

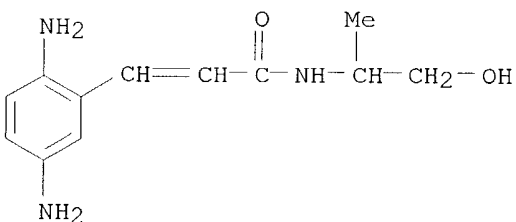
RN 460083-63-0 HCA

CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(1-methylethyl)-, monohydrochloride
(9CI) (CA INDEX NAME)



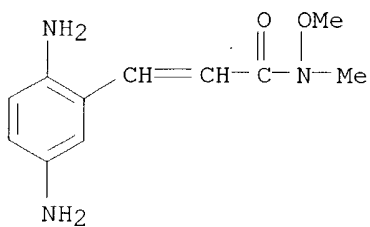
● HCl

RN 460083-64-1 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(2-hydroxy-1-methylethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



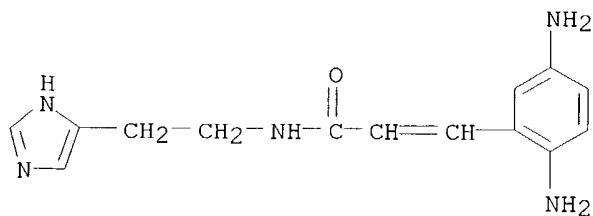
● HCl

RN 460083-65-2 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-methoxy-N-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)



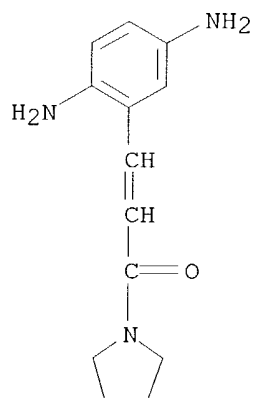
● HCl

RN 460083-66-3 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[2-(1H-imidazol-4-yl)ethyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



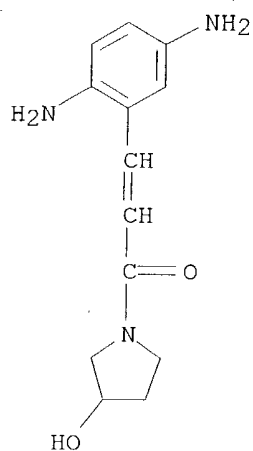
● HCl

RN 460083-67-4 HCA
CN Pyrrolidine, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



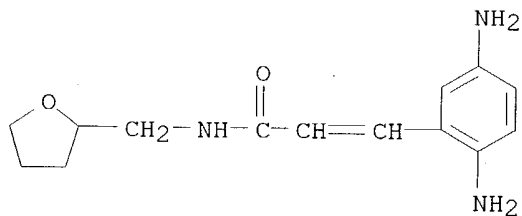
● HCl

RN 460083-69-6 HCA
CN 3-Pyrrolidinol, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



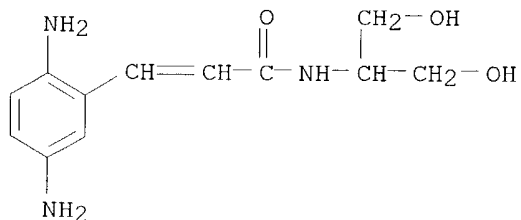
● HCl

RN 460083-72-1 HCA
 CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[(tetrahydro-2-furanyl)methyl]-,
 monohydrochloride (9CI) (CA INDEX NAME)



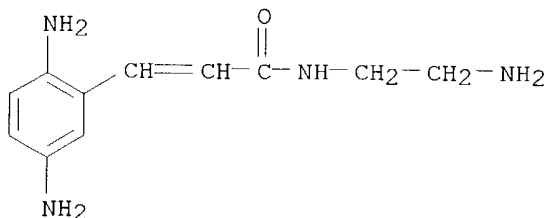
● HCl

RN 460083-73-2 HCA
 CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[2-hydroxy-1-(hydroxymethyl)ethyl]-,
 monohydrochloride (9CI) (CA INDEX NAME)



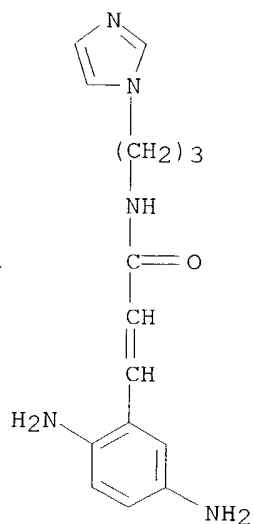
● HCl

RN 460083-74-3 HCA
CN 2-Propenamide, N-(2-aminoethyl)-3-(2,5-diaminophenyl)-, monohydrochloride
(9CI) (CA INDEX NAME)



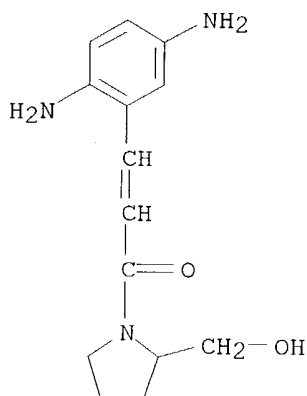
● HCl

RN 460083-75-4 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[3-(1H-imidazol-1-yl)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



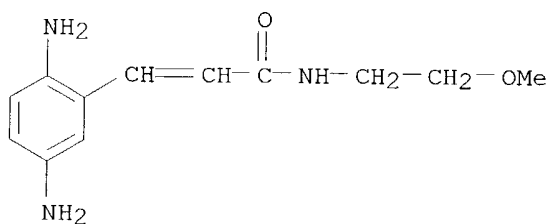
● HCl

RN 460083-76-5 HCA
CN 2-Pyrrolidinemethanol, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



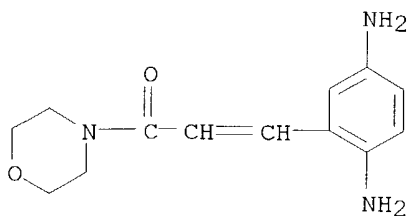
● HCl

RN 460083-77-6 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-(2-methoxyethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

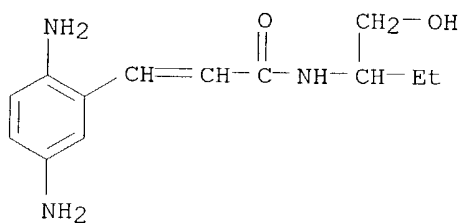
RN 460083-78-7 HCA
CN Morpholine, 4-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride
(9CI) (CA INDEX NAME)



● HCl

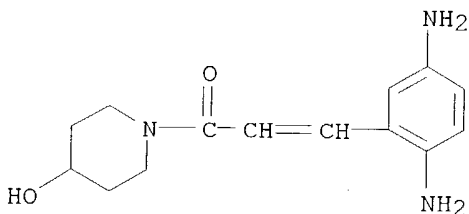
RN 460083-80-1 HCA

CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[1-(hydroxymethyl)propyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



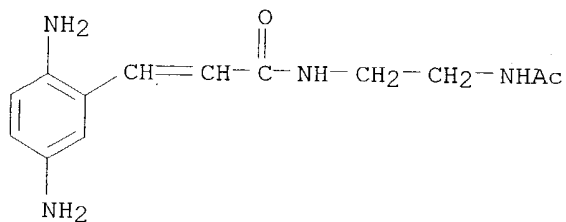
● HCl

RN 460083-81-2 HCA
CN 4-Piperidinol, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



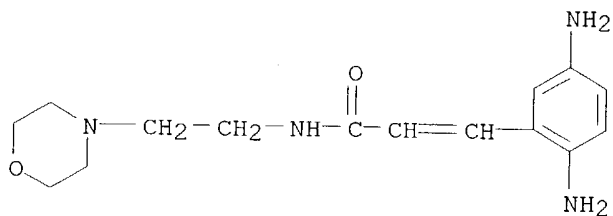
● HCl

RN 460083-82-3 HCA
CN 2-Propenamide, N-[2-(acetylamino)ethyl]-3-(2,5-diaminophenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

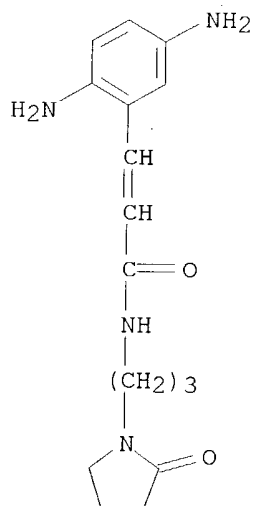
RN 460083-83-4 HCA
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[2-(4-morpholinyl)ethyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460083-84-5 HCA

CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[3-(2-oxo-1-pyrrolidinyl)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



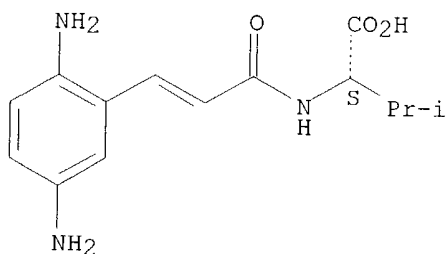
● HCl

RN 460083-85-6 HCA

CN L-Valine, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

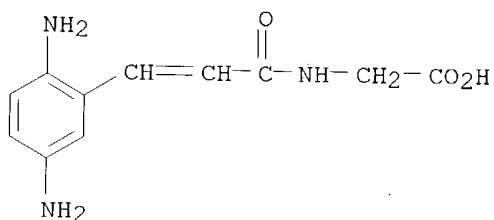
Absolute stereochemistry.

Double bond geometry unknown.



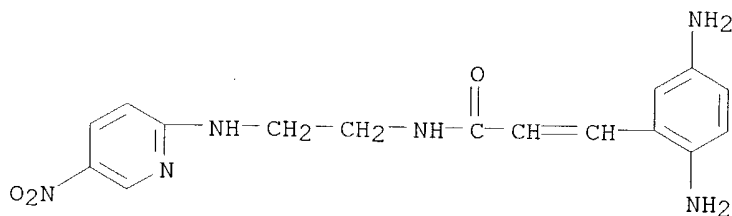
● HCl

RN 460083-86-7 HCA
 CN Glycine, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride
 (9CI) (CA INDEX NAME)



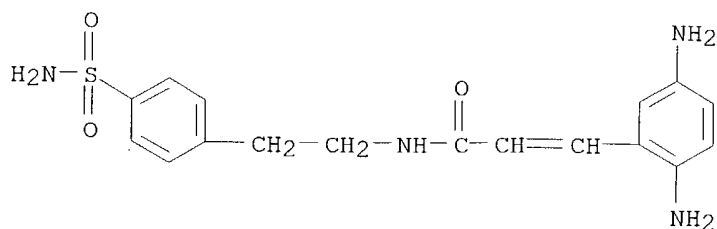
● HCl

RN 460083-87-8 HCA
 CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[2-[(5-nitro-2-pyridinyl)amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460083-88-9 HCA
 CN 2-Propenamide, N-[2-[4-(aminosulfonyl)phenyl]ethyl]-3-(2,5-diaminophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460083-92-5 HCA

CN L-Glutamic acid, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

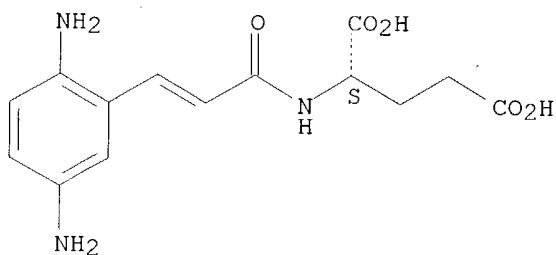
CM 1

CRN 460083-91-4

CMF C14 H17 N3 O5

Absolute stereochemistry.

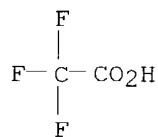
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 460083-94-7 HCA

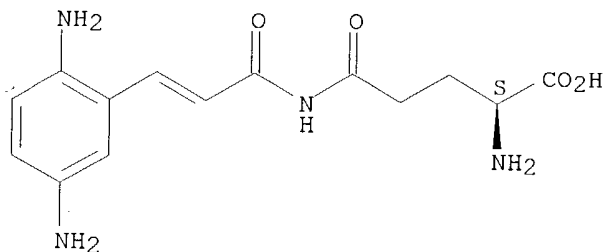
CN L-Glutamine, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 460083-93-6

CMF C14 H18 N4 O4

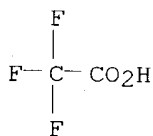
Absolute stereochemistry.
Double bond geometry unknown.



CM 2

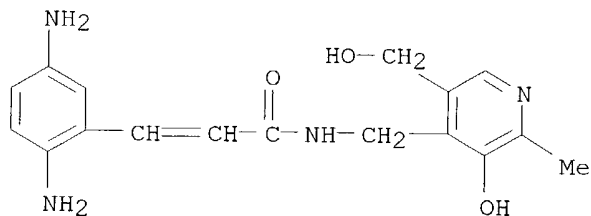
CRN 76-05-1

CMF C2 H F3 O2



RN 460083-97-0 HCA

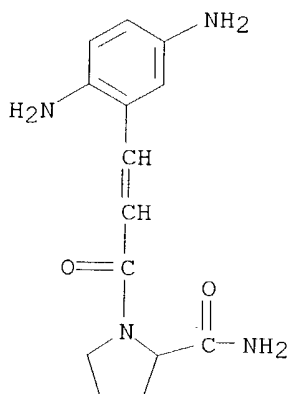
CN 2-Propenamide, 3-(2,5-diaminophenyl)-N-[[3-hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

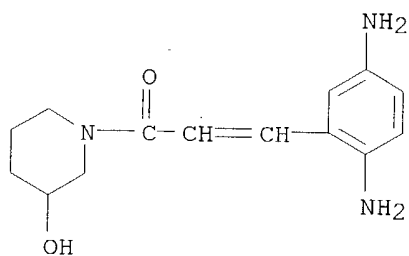
RN 460083-99-2 HCA

CN 2-Pyrrolidinecarboxamide, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



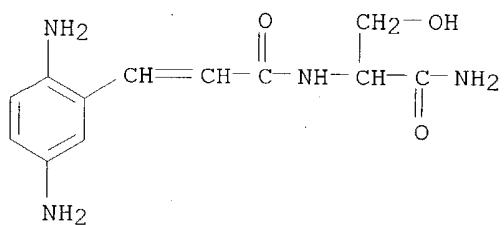
● HCl

RN 460084-00-8 HCA
 CN 3-Piperidinol, 1-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460084-01-9 HCA
 CN 2-Propenamide, N-[2-amino-1-(hydroxymethyl)-2-oxoethyl]-3-(2,5-diaminophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 460084-03-1 HCA

CN L-Aspartic acid, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

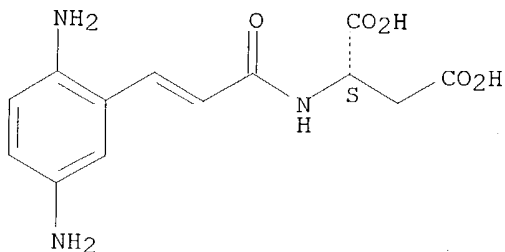
CM 1

CRN 460084-02-0

CMF C13 H15 N3 O5

Absolute stereochemistry.

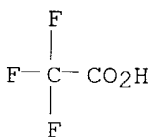
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 460084-05-3 HCA

CN L-Asparagine, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

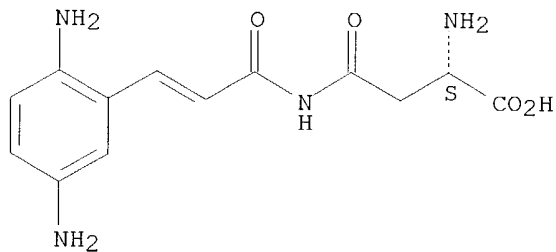
CM 1

CRN 460084-04-2

CMF C13 H16 N4 O4

Absolute stereochemistry.

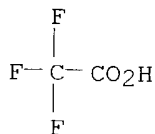
Double bond geometry unknown.



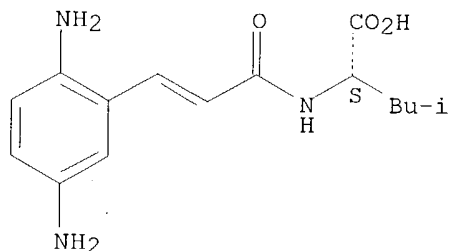
CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 460084-07-5 HCA

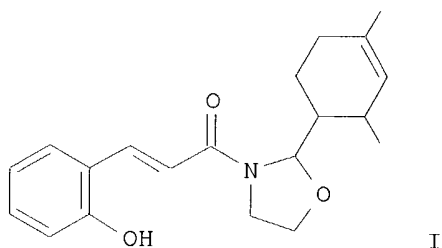
CN L-Leucine, N-[3-(2,5-diaminophenyl)-1-oxo-2-propenyl]-, monohydrochloride
(9CI) (CA INDEX NAME)Absolute stereochemistry.
Double bond geometry unknown.

● HCl

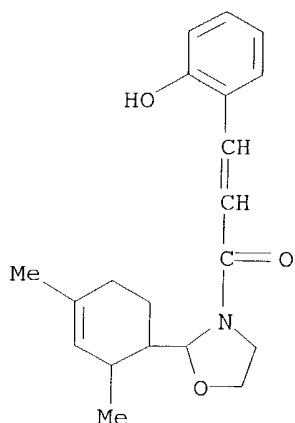
L57 ANSWER 4 OF 15 HCA COPYRIGHT 2004 ACS on STN

136:390775 Photolabile pro-fragrance conjugates. Dykstra, Robert Richard; Miracle, Gregory Scot; Gray, Lon Montgomery (The Procter & Gamble Company, USA). PCT Int. Appl. WO 2002038120 A1 20020516, 64 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US43843 20011106. PRIORITY: US 2000-PV246811 20001108.

GI

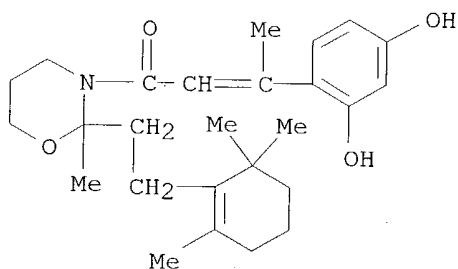


- AB The present invention relates to photolabile pro-fragrance conjugates comprising: a photo-labile unit which upon exposure to electromagnetic radiation is capable of releasing a pro-fragrance unit; and a pro-fragrance unit, which when so released is either a pro-fragrance compound capable of releasing a fragrance raw material; or a fragrance raw material. The present invention relates to systems for delivering fragrances to a situs, and to laundry detergent compns., fine fragrances, personal care and hair care compns. comprising said systems. One examples compound prepared was a triplal oxazolidine conjugate (I).
- IC ICM A61K007-46
ICS C11D003-50; C07C225-22; C07C233-01
- CC 62-5 (Essential Oils and Cosmetics)
Section cross-reference(s): 25, 28, 30
- IT Odor and Odorous substances
Perfumes
Photolysis
(photolabile pro-fragrance conjugates)
- IT 425386-63-6P 425386-65-8P 425386-67-0P
425386-71-6P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(photolabile pro-fragrance conjugates)
- IT 425386-63-6P 425386-65-8P 425386-67-0P
425386-71-6P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(photolabile pro-fragrance conjugates)
- RN 425386-63-6 HCA
- CN Oxazolidine, 2-(2,4-dimethyl-3-cyclohexen-1-yl)-3-[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



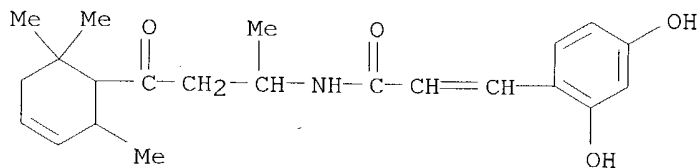
RN 425386-65-8 HCA

CN 2H-1,3-Oxazine, 3-[3-(2,4-dihydroxyphenyl)-1-oxo-2-butenyl]tetrahydro-2-methyl-2-[2-(2,6,6-trimethyl-1-cyclohexen-1-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 425386-67-0 HCA

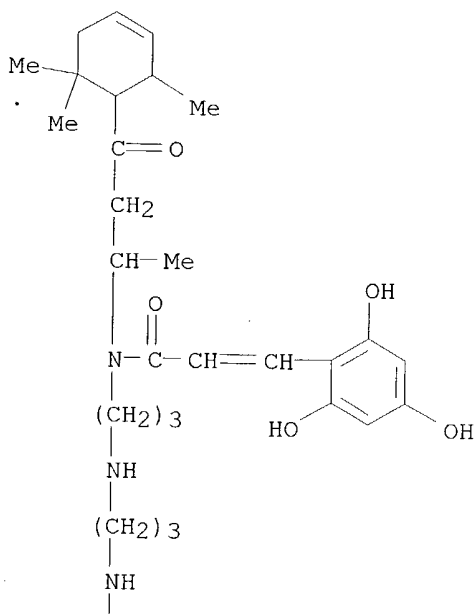
CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-[1-methyl-3-oxo-3-(2,6,6-trimethyl-3-cyclohexen-1-yl)propyl]- (9CI) (CA INDEX NAME)



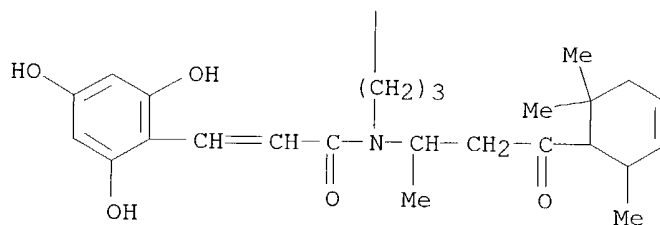
RN 425386-71-6 HCA

CN 2-Propenamide, N,N'-[1,3-propanediylbis(imino-3,1-propanediyl)]bis[N-[1-methyl-3-oxo-3-(2,6,6-trimethyl-3-cyclohexen-1-yl)propyl]-3-(2,4,6-trihydroxyphenyl)- (9CI) (CA INDEX NAME)

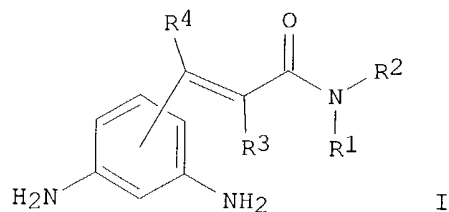
PAGE 1-A



PAGE 2-A



L57 ANSWER 5 OF 15 HCA COPYRIGHT 2004 ACS on STN
 135:288588 (m-Diaminophenyl)acrylamide derivatives and hair coloring agents
 containing these compounds. (Wella AG, Germany). Ger.
 Gebrauchsmusterschrift DE 20111037 U1 20011004, 48 pp. (German). CODEN:
 GGXXFR. APPLICATION: DE 2001-20111037 20010704.
 GI



AB (m-Diaminophenyl)acrylamide derivs. I [R1, R2 = H, C1-2 alkoxy, C1-6 alkyl, unsatd. C3-6 alkyl, C2-4 hydroxyalkyl, C3-4 dihydroxyalkyl, C2-4 aminoalkyl, a C2-4 dimethylaminoalkyl, C2-4 acetylaminoalkyl, a C2-4 methoxyalkyl, C2-4 ethoxyalkyl, C1-4 cyanoalkyl, C1-4 carboxyalkyl, C2-4 aminocarbonylalkyl, pyridylmethyl, furfuryl, hydrogenated furfuryl, substituted pyridyl, (un)substituted Et, (un)substituted Ph, substituted aminopyrazolyl; or R1 and R2 together with the N atom form a ring; R3, R4 = H, C1-4 alkyl; preferably, R3 = R4 = H, or R1, R2 and R4 = H, R2 = aminophenyl, hydroxyphenyl] or their physiol. compatible, water-soluble salts, useful in oxidative hair dyes based on a developer substance-coupling substance combination in one suitable cosmetic carrier, are claimed. Preferred compds. I are 3-(2,4-diaminophenyl)-1-morpholinopropenone, 3-(2,4-diaminophenyl)-N-(4-hydroxyphenyl)acrylamide, 3-(3,5-diaminophenyl)-N-(4-hydroxyphenyl)acrylamide, N-(3-aminophenyl)-3-(3,5-diaminophenyl)acrylamide and N-(4-aminophenyl)-3-(3,5-diaminophenyl)acrylamide, or their physiol. acceptable salts (prepn. given). In examples given, compds. I are formulated with one or more known developer substances and one or more known addnl. coupling substances to give various shades of color when applied to hair; e.g., 0.10 g 3-(2,4-diaminophenyl)-1-morpholinopropenone HCl salt, 0.30 g 1,4-diaminobenzene, 0.05 g 1,3-diamino-4-(2-hydroxyethyl)aminoaniline sulfate, and 0.05 g 3-aminophenol (formulation given) afforded blond hair.

IC ICM C07C237-20

ICS A61K007-13; C07D317-48; C07D295-04

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 62

IT **364343-44-2P 364343-45-3P 364343-46-4P**

364343-47-5P 364343-48-6P 364343-49-7P 364343-50-0P

364343-51-1P 364343-52-2P **364343-53-3P**

364343-54-4P 364343-55-5P **364343-56-6P** 364343-57-7P

364343-58-8P 364343-59-9P 364343-60-2P 364343-61-3P 364343-62-4P

364343-63-5P 364343-64-6P 364343-65-7P 364343-66-8P 364343-67-9P

364343-68-0P 364343-69-1P 364343-70-4P 364343-71-5P 364343-72-6P

364343-73-7P 364343-74-8P 364343-75-9P 364343-76-0P 364343-77-1P

364343-78-2P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation for use as coupling substance component in oxidative hair dye based on developer-coupling substance combination)

IT **364343-39-5P** 364343-40-8P 364343-41-9P 364343-42-0P
364343-43-1P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

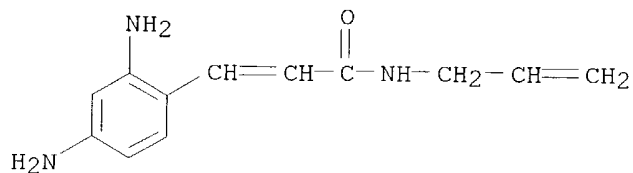
(preparation for use as coupling substance component in oxidative hair dye based on developer-coupling substance combination containing (diaminophenyl)acrylamide derivs.)

IT 364343-44-2P 364343-45-3P 364343-46-4P
364343-47-5P 364343-51-1P 364343-53-3P
364343-54-4P 364343-56-6P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(preparation for use as coupling substance component in oxidative hair dye
based on developer-coupling substance combination)

RN 364343-44-2 HCA

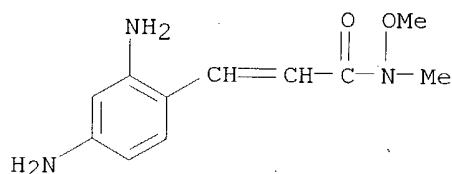
CN 2-Propenamide, 3-(2,4-diaminophenyl)-N-2-propenyl-, hydrochloride (9CI)
(CA INDEX NAME)



● x HCl

RN 364343-45-3 HCA

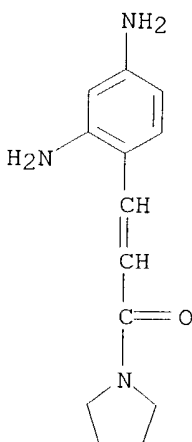
CN 2-Propenamide, 3-(2,4-diaminophenyl)-N-methoxy-N-methyl-, hydrochloride
(9CI) (CA INDEX NAME)



● x HCl

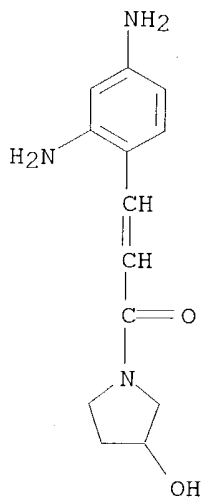
RN 364343-46-4 HCA

CN Pyrrolidine, 1-[3-(2,4-diaminophenyl)-1-oxo-2-propenyl]-, hydrochloride
(9CI) (CA INDEX NAME)



● x HCl

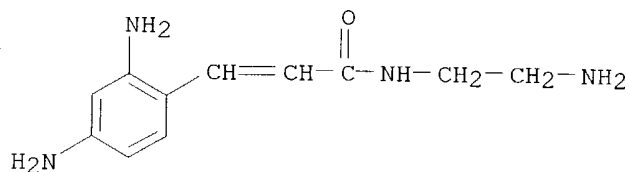
RN 364343-47-5 HCA

CN 3-Pyrrolidinol, 1-[3-(2,4-diaminophenyl)-1-oxo-2-propenyl]-, hydrochloride
(9CI) (CA INDEX NAME)

● x HCl

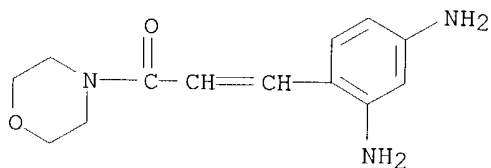
RN 364343-51-1 HCA

CN 2-Propenamamide, N-(2-aminoethyl)-3-(2,4-diaminophenyl)-, hydrochloride
(9CI) (CA INDEX NAME)



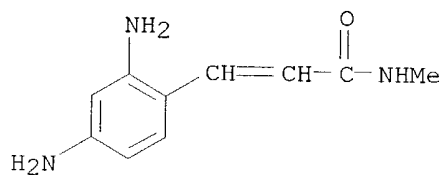
●x HCl

RN 364343-53-3 HCA
CN Morpholine, 4-[3-(2,4-diaminophenyl)-1-oxo-2-propenyl]-, hydrochloride
(9CI) (CA INDEX NAME)



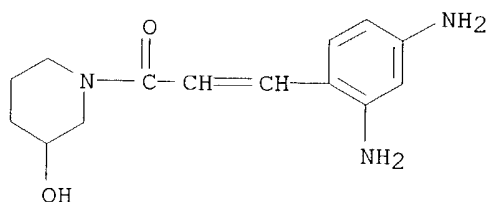
●x HCl

RN 364343-54-4 HCA
CN 2-Propenamide, 3-(2,4-diaminophenyl)-N-methyl-, hydrochloride (9CI) (CA
INDEX NAME)



●x HCl

RN 364343-56-6 HCA
CN 3-Piperidinol, 1-[3-(2,4-diaminophenyl)-1-oxo-2-propenyl]-, hydrochloride
(9CI) (CA INDEX NAME)



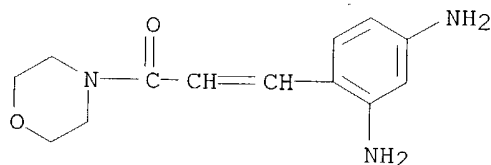
● x HCl

IT **364343-39-5P**

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation for use as coupling substance component in oxidative hair dye based on developer-coupling substance combination containing (diaminophenyl)acrylamide derivs.)

RN 364343-39-5 HCA

CN Morpholine, 4-[3-(2,4-diaminophenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



L57 ANSWER 6 OF 15 HCA COPYRIGHT 2004 ACS on STN

134:147736 Synthetic analogues to the spermidine-spermine alkaloid tenuilobine. Popaj, Kasim; Guggisberg, Armin; Hesse, Manfred (Organisch-chemisches Institut der Universitat Zurich, Zurich, CH-8057, Switz.). Helvetica Chimica Acta, 83(11), 3021-3034 (English) 2000. CODEN: HCACAV. ISSN: 0018-019X. OTHER SOURCES: CASREACT 134:147736. Publisher: Verlag Helvetica Chimica Acta.

AB Naturally occurring spider and wasp toxins are potent inhibitors of glutamate receptors in the central nervous system. They consist of a polyamine backbone and carboxylic acids or amino acids linked by peptide bonds. In some respects, the plant alkaloid tenuilobine, a derivative of spermine and spermidine, shows structural similarities to these toxins. In the present paper, the synthesis of the five tenuilobine analogs is described. These derivs. differ in their **aromatic** carboxylic acid subunits and in the polyamine moiety.

CC 31-6 (Alkaloids)

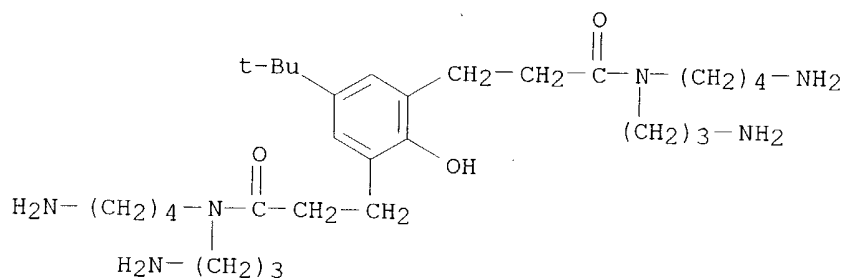
IT 20490-18-0P 34911-36-9P 94374-53-5P 322638-48-2P 322638-49-3P
322638-50-6P 322638-51-7P 322638-52-8P **322638-53-9P**
322638-56-2P 322638-58-4P 322638-60-8P 322638-61-9P
322638-62-0P 322638-63-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthetic analogs to the spermidine-spermine alkaloid tenuilobine)

IT **322638-54-0P 322638-55-1P 322638-57-3P**
322638-59-5P 322638-64-2P 322638-65-3P

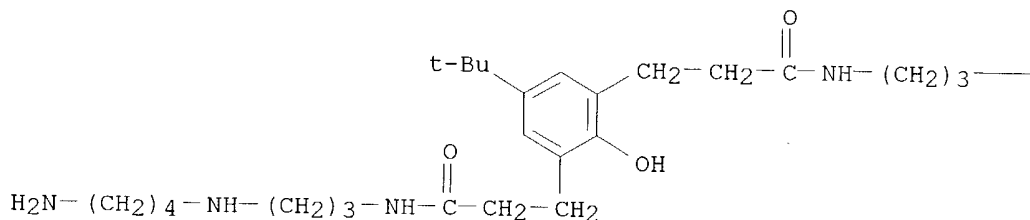
RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthetic analogs to the spermidine-spermine alkaloid tenuilobine)
 IT **322638-53-9P 322638-56-2P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthetic analogs to the spermidine-spermine alkaloid tenuilobine)
 RN 322638-53-9 HCA
 CN 1,3-Benzenedipropanamide, N,N'-bis(4-aminobutyl)-N,N'-bis(3-aminopropyl)-5-(1,1-dimethylethyl)-2-hydroxy-, tetrahydrochloride (9CI) (CA INDEX NAME)



● 4 HCl

RN 322638-56-2 HCA
 CN 1,3-Benzenedipropanamide, N,N'-bis[3-[(4-aminobutyl)amino]propyl]-5-(1,1-dimethylethyl)-2-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A

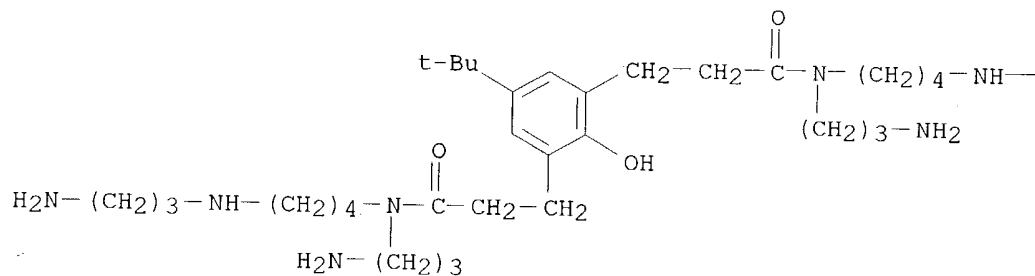


PAGE 1-B

—NH—(CH₂)₄—NH₂

IT **322638-54-0P 322638-55-1P 322638-57-3P**
322638-59-5P 322638-64-2P 322638-65-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthetic analogs to the spermidine-spermine alkaloid tenuilobine)
 RN 322638-54-0 HCA
 CN 1,3-Benzenedipropanamide, N,N'-bis(3-aminopropyl)-N,N'-bis[4-[(3-aminopropyl)amino]butyl]-5-(1,1-dimethylethyl)-2-hydroxy- (9CI) (CA INDEX NAME)

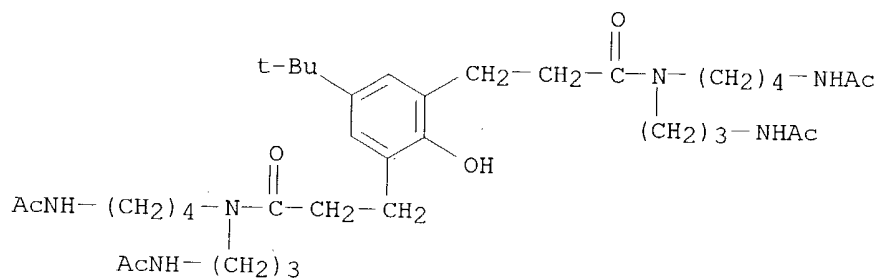
PAGE 1-A



PAGE 1-B

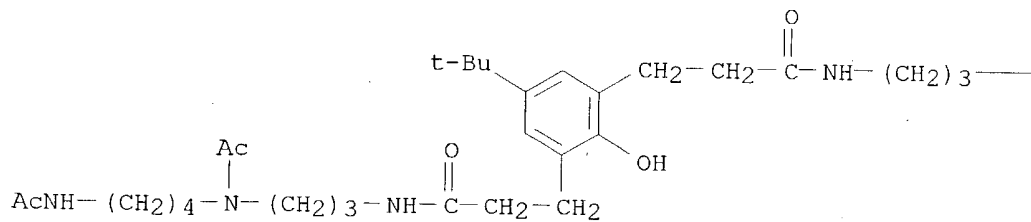
— $(\text{CH}_2)_3-\text{NH}_2$

RN 322638-55-1 HCA
 CN 1,3-Benzenedipropylamine, N,N'-bis[4-(acetylamino)butyl]-N,N'-bis[3-(acetylamino)propyl]-5-(1,1-dimethylethyl)-2-hydroxy- (9CI) (CA INDEX NAME)

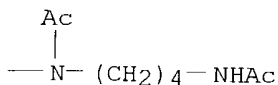


RN 322638-57-3 HCA
 CN 1,3-Benzenedipropylamine, N,N'-bis[3-[acetyl[4-(acetylamino)butyl]amino]propyl]-5-(1,1-dimethylethyl)-2-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



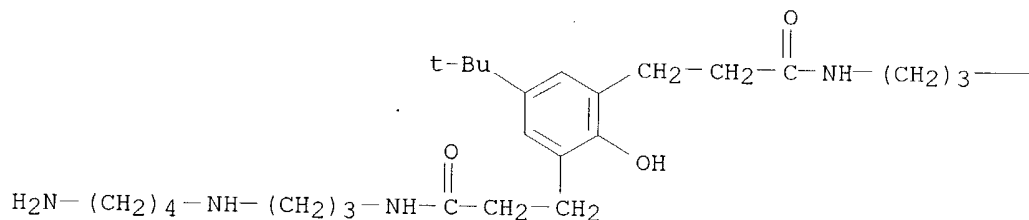
PAGE 1-B



RN 322638-59-5 HCA

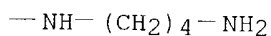
CN 1,3-Benzenedipropanamide, N,N'-bis[3-[(4-aminobutyl)amino]propyl]-5-(1,1-dimethylethyl)-2-hydroxy-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



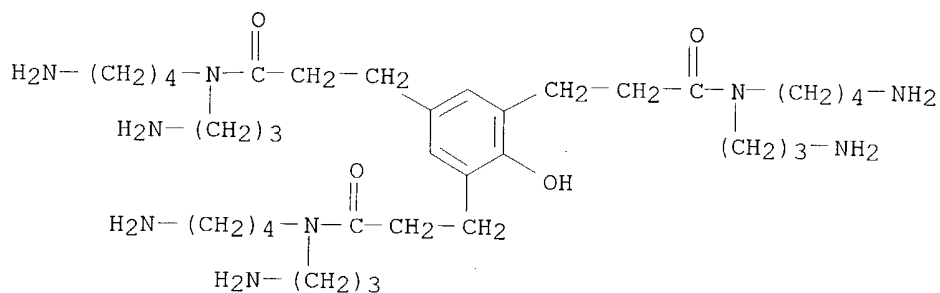
● 4 HCl

PAGE 1-B



RN 322638-64-2 HCA

CN 1,3,5-Benzenetripropanamide, N,N',N''-tris(4-aminobutyl)-N,N',N''-tris(3-aminopropyl)-2-hydroxy-, tetrahydrochloride (9CI) (CA INDEX NAME)

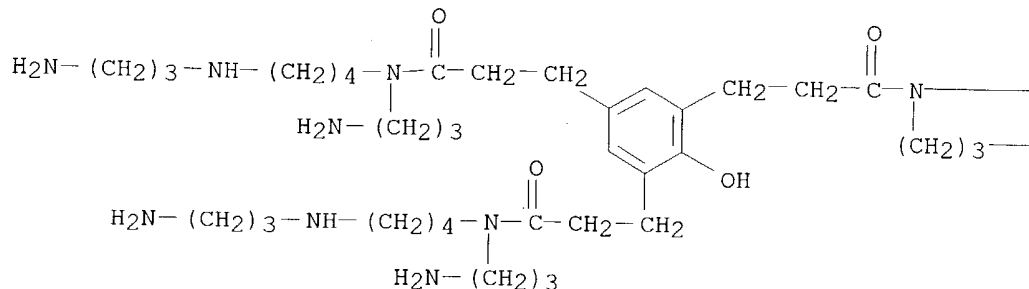


● 4 HCl

RN 322638-65-3 HCA

CN 1,3,5-Benzenetripropanamide, N,N',N''-tris(3-aminopropyl)-N,N',N''-tris[4-[(3-aminopropyl)amino]butyl]-2-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



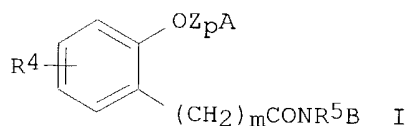
PAGE 1-B

— (CH₂)₄—NH—(CH₂)₃—NH₂

— NH₂

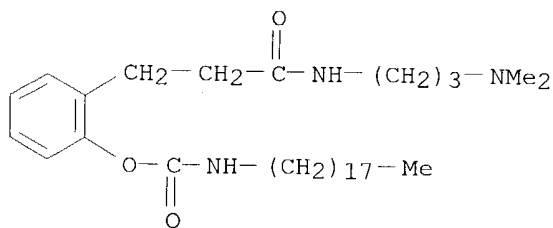
L57 ANSWER 7 OF 15 HCA COPYRIGHT 2004 ACS on STN
133:150582 Preparation of 1-aminocarbonylalkyl-2-aminocarbonyloxybenzenes and related compounds as hair growth promoters.. Kobayashi, Koji; Fukunishi, Hirotada; Iwabuchi, Tokuro (Shiseido Co., Ltd., Japan). Eur. Pat. Appl. EP 1026150 A1 20000809, 61 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2000-102128 20000204. PRIORITY: JP 1999-27604 19990204.

GI

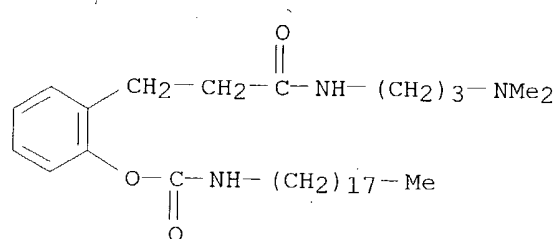


AB Title compds. [I; A = R1, B = (CH₂)_nNR₂R₃ or vice versa; Z = CO, CONR₆; R₁ = hydrocarbyl; R₂, R₃ = H, alkyl, PhCH₂; NR₂R₃ = heterocyclyl; R₄ = H, halo, alkyl, acyl, NO₂, cyano, alkoxy, carbamoyl, alkylcarbamoyl, alkylamino, acylamino, alkoxy, acyloxy; R₆ = H, alkyl, acyl, alkylcarbamoyl; when B = (CH₂)_nNR₂R₃ or when ZpA = CONR₆(CH₂)_nNR₂R₃, CONR₅(CH₂)_nNR₂R₃ and CONR₆(CH₂)_nNR₂R₃ can = CONYNR₂; NYN = atoms to form a 6-7 membered heterocycle; p = 0, 1; m = 1, 2; n = 0-5], were prepared Thus, Et₃N, octadecyl isocyanate, and 3-(2-hydroxyphenyl)-1-(4-methylpiperazino)-1-propanone were stirred in CH₂Cl₂ to give 2-[3-(4-methylpiperazino)-3-oxopropyl]phenyl N-octadecylcarbamate. The latter as a 0.1% solution applied

- to shaved mice gave 100% hair regrowth after 24 days.
- IC ICM C07C235-34
ICS C07C271-44; C07C271-52; C07D295-13; C07D295-182; C07D295-205;
C07D295-088; A61K007-06; A61K007-48
- CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25, 62
- IT 287199-06-8P 287199-07-9P 287199-08-0P
287199-09-1P 287199-10-4P 287199-11-5P
287199-12-6P 287199-13-7P 287199-14-8P 287199-15-9P 287199-16-0P
287199-17-1P 287199-18-2P 287199-19-3P
287199-20-6P 287199-21-7P 287199-22-8P 287199-23-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-aminocarbonylalkyl-2-aminocarbonyloxybenzenes and related compds. as hair growth promoters)
- IT 287199-24-0P 287199-25-1P 287199-26-2P
287199-27-3P 287199-28-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-aminocarbonylalkyl-2-aminocarbonyloxybenzenes and related compds. as hair growth promoters)
- IT 287199-06-8P 287199-07-9P 287199-08-0P
287199-09-1P 287199-10-4P 287199-11-5P
287199-18-2P 287199-19-3P 287199-20-6P
287199-21-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-aminocarbonylalkyl-2-aminocarbonyloxybenzenes and related compds. as hair growth promoters)
- RN 287199-06-8 HCA
- CN Carbamic acid, octadecyl-, 2-[3-[[3-(dimethylamino)propyl]amino]-3-oxopropyl]phenyl ester (9CI) (CA INDEX NAME)



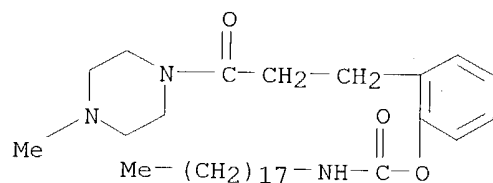
- RN 287199-07-9 HCA
- CN Carbamic acid, octadecyl-, 2-[3-[[3-(dimethylamino)propyl]amino]-3-oxopropyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

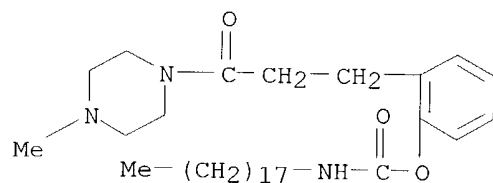
RN 287199-08-0 HCA

CN Carbamic acid, octadecyl-, 2-[3-(4-methyl-1-piperazinyl)-3-oxopropyl]phenyl ester (9CI) (CA INDEX NAME)



RN 287199-09-1 HCA

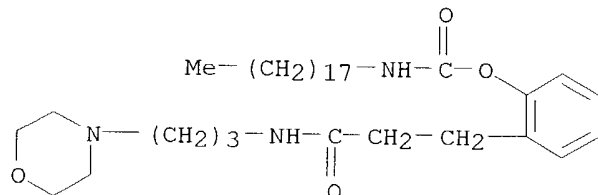
CN Carbamic acid, octadecyl-, 2-[3-(4-methyl-1-piperazinyl)-3-oxopropyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

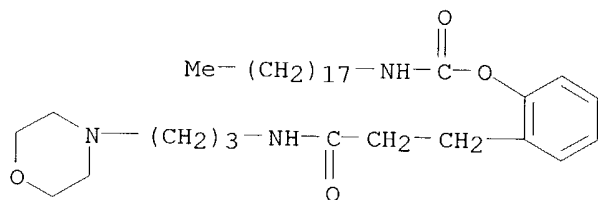
RN 287199-10-4 HCA

CN Carbamic acid, octadecyl-, 2-[3-[[3-(4-morpholinyl)propyl]amino]-3-oxopropyl]phenyl ester (9CI) (CA INDEX NAME)



RN 287199-11-5 HCA

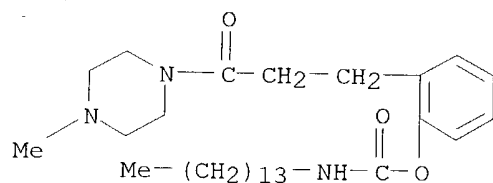
CN Carbamic acid, octadecyl-, 2-[3-[[3-(4-morpholinyl)propyl]amino]-3-oxopropyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

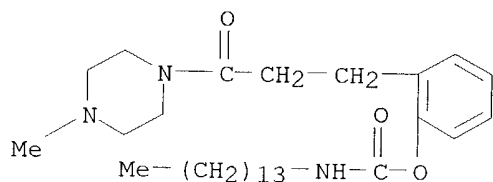
RN 287199-18-2 HCA

CN Carbamic acid, tetradecyl-, 2-[3-(4-methyl-1-piperazinyl)-3-oxopropyl]phenyl ester (9CI) (CA INDEX NAME)



RN 287199-19-3 HCA

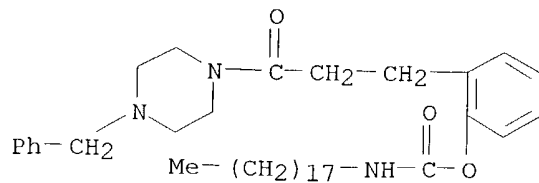
CN Carbamic acid, tetradecyl-, 2-[3-(4-methyl-1-piperazinyl)-3-oxopropyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

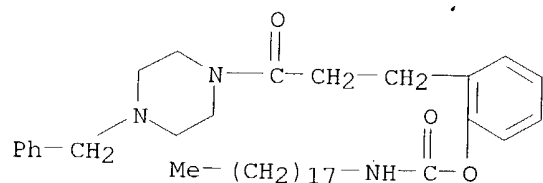
RN 287199-20-6 HCA

CN Carbamic acid, octadecyl-, 2-[3-oxo-3-[4-(phenylmethyl)-1-piperazinyl]propyl]phenyl ester (9CI) (CA INDEX NAME)



RN 287199-21-7 HCA

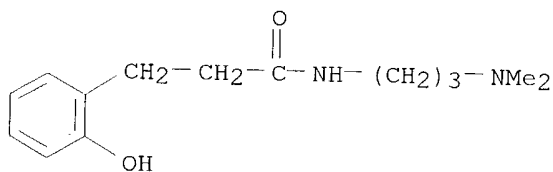
CN Carbamic acid, octadecyl-, 2-[3-oxo-3-[4-(phenylmethyl)-1-piperazinyl]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



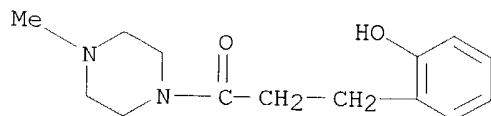
● HCl

IT 287199-24-0P 287199-25-1P 287199-26-2P
287199-27-3PRL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)(preparation of 1-aminocarbonylalkyl-2-aminocarbonyloxybenzenes and related
comps. as hair growth promoters)

RN 287199-24-0 HCA

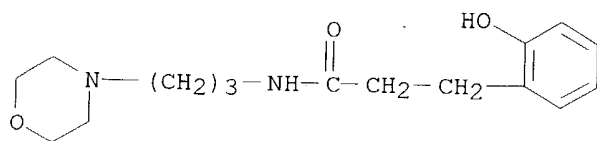
CN Benzenepropanamide, N-[3-(dimethylamino)propyl]-2-hydroxy- (9CI) (CA
INDEX NAME)

RN 287199-25-1 HCA

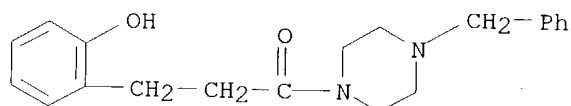
CN Piperazine, 1-[3-(2-hydroxyphenyl)-1-oxopropyl]-4-methyl- (9CI) (CA INDEX
NAME)

RN 287199-26-2 HCA

CN Benzenepropanamide, 2-hydroxy-N-[3-(4-morpholinyl)propyl]- (9CI) (CA
INDEX NAME)



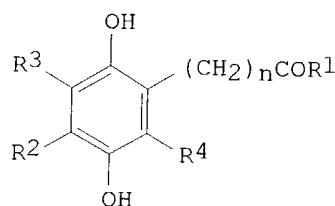
RN 287199-27-3 HCA

CN Piperazine, 1-[3-(2-hydroxyphenyl)-1-oxopropyl]-4-(phenylmethyl)- (9CI)
(CA INDEX NAME)

L57 ANSWER 8 OF 15 HCA COPYRIGHT 2004 ACS on STN

118:197805 Preparation of (2,5-dihydroxyphenyl)carboxylates, as skin-lightening agents.. Junino, Alex; Lagrange, Alain; Nguyen Quang Lan; Bourboulon, Marie Alix (Oreal S. A., Fr.). Eur. Pat. Appl. EP 526302 A1 19930203, 14 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, PT, SE. (French). CODEN: EPXXDW. APPLICATION: EP 1992-402078 19920717. PRIORITY: FR 1991-9029 19910717.

GI



I

AB Cosmetic compns. containing 2,5-dihydroxyphenylcarboxylic acids [I; R1 = OH, OR5 (R5 = C1-20 alkyl, C2-20 alkenyl etc.); R2, R3 = H, C1-4 alkyl, C1-4 alkoxy; R4 = H, C1-4 alkyl; n = 0-20] (preparation given) are used for skin depigmentation. A mixture of 2,5-dihydroxy-4-methylphenylacetic acid (II) and a sulfonic acid resin (IRN-77R) in absolute MeOH was refluxed to obtain II Me ester (III). A cosmetic lotion contained EtOH 50, PEG 30, ethoxydiglycol 5, glycerin 5, III 3.6 and water to 100 g.

IC ICM A61K007-48

ICS C07C069-732; C07C235-34

CC 62-4 (Essential Oils and Cosmetics)

Section cross-reference(s): 25

IT 2413-20-9P 2901-94-2P 2901-95-3P 3209-15-2P 3899-19-2P
5981-37-3P 10538-47-3P, 2,5-Dihydroxyphenyl propionic acid 13618-45-6P
20452-54-4P 29235-44-7P 29865-98-3P, 2,5-Dihydroxy-4-methoxy phenyl
acetic acid 36469-53-1P 42604-28-4P 42604-30-8P 42604-39-7P
54637-01-3P 61654-77-1P 67405-55-4P 70318-70-6P 70318-72-8P
70318-76-2P 74587-23-8P 74712-94-0P 77220-20-3P 77267-97-1P
77800-55-6P 105476-09-3P 106296-33-7P 106296-36-0P 116058-73-2P
128760-84-9P 146803-71-6P 146803-72-7P 146803-73-8P

146803-74-9P 146803-75-0P 146803-76-1P 146803-77-2P 146803-78-3P
146803-79-4P 146803-80-7P 146803-81-8P 146803-82-9P 146803-83-0P
146803-84-1P

RL: PREP (Preparation)

(preparation of, as skin-depigmentation agent, for cosmetics)

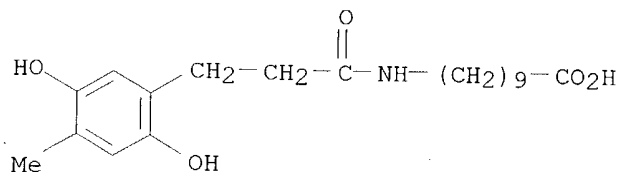
IT **146803-73-8P**

RL: PREP (Preparation)

(preparation of, as skin-depigmentation agent, for cosmetics)

RN 146803-73-8 HCA

CN Decanoic acid, 10-[[3-(2,5-dihydroxy-4-methylphenyl)-1-oxopropyl]amino]-
(9CI) (CA INDEX NAME)



L57 ANSWER 9 OF 15 HCA COPYRIGHT 2004 ACS on STN

118:146573 Browning inhibitors for foods and beverages. McEvily, Arthur J.;
Iyengar, Radha; Gross, Akiva (Opta Food Ingredients, Inc., USA). PCT Int.
Appl. WO 9222213 A1 19921223, 27 pp. DESIGNATED STATES: W: CA, JP; RW:
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE. (English).
CODEN: PIXXD2. APPLICATION: WO 1992-US4867 19920610. PRIORITY: US
1991-712794 19910610.

AB Substituted resorcinol derivs. and an additive selected from a sulfite,
chelating agent, acidulant, and/or an inorg. salt are used to prevent
browning of food. The compns. are useful for prevention of enzymic
browning of food associated with tyrosinase and do not degrade the
organoleptic characteristics of the foods.

IC ICM A23B007-00

CC 17-4 (Food and Feed Chemistry)

IT 108-46-3D, Resorcinol, derivs. 136-77-6 5631-68-5 **145903-85-1**
145903-86-2 145903-87-3

RL: BIOL (Biological study)

(for prevention of enzymic browning of foods)

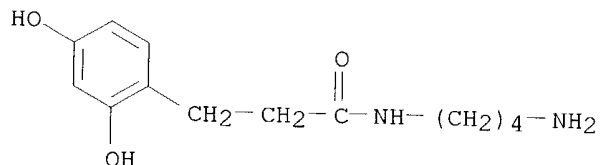
IT **145903-85-1 145903-86-2 145903-87-3**

RL: BIOL (Biological study)

(for prevention of enzymic browning of foods)

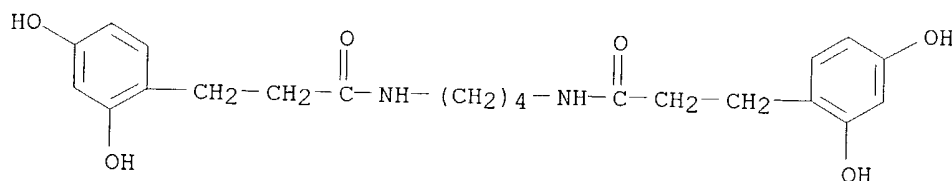
RN 145903-85-1 HCA

CN Benzenepropanamide, N-(4-aminobutyl)-2,4-dihydroxy- (9CI) (CA INDEX NAME)



RN 145903-86-2 HCA

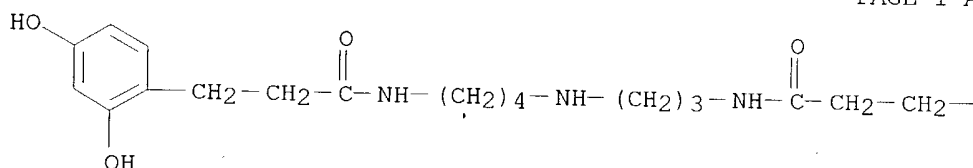
CN Benzenepropanamide, N,N'-1,4-butanediylbis[2,4-dihydroxy- (9CI) (CA INDEX NAME)



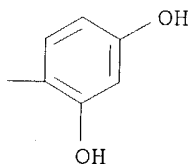
RN 145903-87-3 HCA

CN Benzenepropanamide, N-[3-[[4-[[3-(2,4-dihydroxyphenyl)-1-oxopropyl]amino]butyl]amino]propyl]-2,4-dihydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L57 ANSWER 10 OF 15 HCA COPYRIGHT 2004 ACS on STN

118:100623 Inhibition of polyphenol oxidase by phenolic compounds. McEvily, A. J.; Iyengar, R.; Gross, A. T. (Opta Food Ingredients, Inc., Cambridge, MA, 02139, USA). ACS Symposium Series, 506(Phenolic Compd. Food Their Eff. Health I), 318-25 (English) 1992. CODEN: ACSMC8. ISSN: 0097-6156.

AB Several inhibitors of polyphenol oxidase (PPO) were isolated from a fig latex extract. The inhibitors were purified and their relative potencies determined by using com. mushroom PPO in an in vitro assay system. The inhibitors were novel plant secondary metabolites closely related to other phenolic compds. known to play important roles in flowering plants. Structure-activity relationships were studied by using synthetic resorcinol analogs, several of which are potent PPO inhibitors. In addition to the in vitro studies, certain of these compds. inhibit enzymic browning (melanosis) in foods such as shrimp, potatoes, and apples as well as beverages such as grape juice. The inhibitors are water-soluble, stable, effective at low concentration, and have potential as functional alternatives

to

sulfite for the inhibition of melanosis. The chemical nature of the PPO inhibitors, kinetic studies, safety data, and results obtained on foods are discussed.

CC 17-2 (Food and Feed Chemistry)

Section cross-reference(s): 7

IT 89-86-1, 4-Carboxyresorcinol 136-77-6, 4-Hexylresorcinol 151-10-0
500-66-3, 5-Pentylresorcinol 500-67-4, 5-Heptylresorcinol 504-15-4,

5-Methylresorcinol 608-25-3, 2-Methylresorcinol 2138-20-7,
 4-Cyclohexylresorcinol 2896-60-8, 4-Ethylresorcinol 3144-54-5
 3158-56-3, 5-Pentadecylresorcinol 24305-56-4, 4-Dodecylresorcinol
 29554-26-5, Caffeoylputrescine **145903-86-2**

RL: BIOL (Biological study)
 (polyphenol oxidase inhibition by)

IT 5631-68-5 **145903-85-1 145903-87-3**

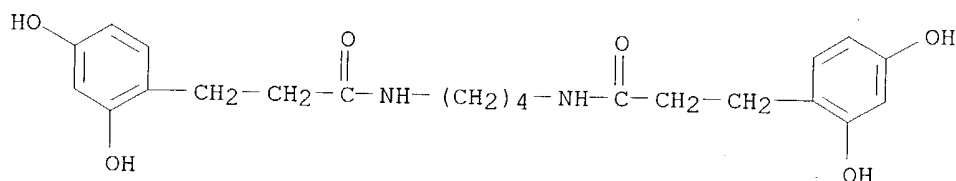
RL: BIOL (Biological study)
 (polyphenol oxidase inhibition by, from fig latex)

IT **145903-86-2**

RL: BIOL (Biological study)
 (polyphenol oxidase inhibition by)

RN 145903-86-2 HCA

CN Benzenepropanamide, N,N'-1,4-butanediylbis[2,4-dihydroxy- (9CI) (CA INDEX NAME)

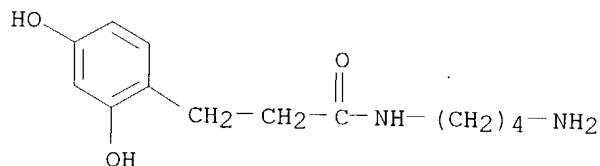


IT **145903-85-1 145903-87-3**

RL: BIOL (Biological study)
 (polyphenol oxidase inhibition by, from fig latex)

RN 145903-85-1 HCA

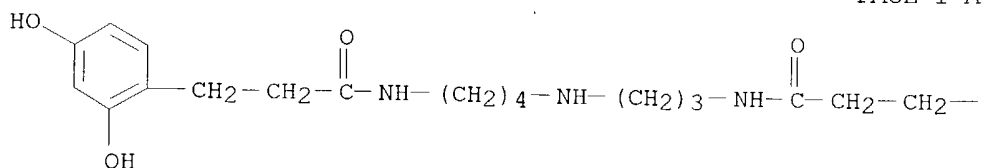
CN Benzenepropanamide, N-(4-aminobutyl)-2,4-dihydroxy- (9CI) (CA INDEX NAME)



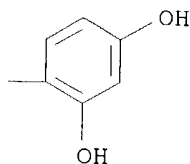
RN 145903-87-3 HCA

CN Benzenepropanamide, N-[3-[[4-[[3-(2,4-dihydroxyphenyl)-1-oxopropyl]amino]butyl]amino]propyl]-2,4-dihydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L57 ANSWER 11 OF 15 HCA COPYRIGHT 2004 ACS on STN

116:256009 Development of potent and selective CCK-A receptor agonists from Boc-CCK-4: tetrapeptides containing Lys(Nε)-amide residues.

Shiosaki, Kazumi; Lin, Chun Wel; Kopecka, Hana; Craig, Richard A.; Bianchi, Bruce R.; Miller, Thomas R.; Witte, David G.; Stashko, Michael; Nadzan, Alex M. (Neurosci. Res. Div., Abbott Lab., Abbott Park, IL, 60064, USA). Journal of Medicinal Chemistry, 35(11), 2007-14 (English) 1992. CODEN: JMCMAR. ISSN: 0022-2623.

AB A series of Boc-CCK-4 (Boc = CO₂CMe₃) derivs. represented by the general structure Boc-Trp-Lys(COR)Asp-Phe-NH₂, where R is an **aromatic**, heterocyclic, or aliphatic group, are potent and selective CCK-A receptor agonists. These amide-bearing compds. complement the previously described urea-based tetrapeptides (Shiosaki et al. 1991); structure activity studies revealed parallel as well as divergent trends between these two series. A significant correlation was observed between pancreatic binding affinity and the resonance constant ρ_{Ph} of the Ph substituent in one particular series of derivs. Sulfation of phenolic amides appended onto the ε-amino group of the lysine did not affect affinity for the CCK-A receptor in contrast to the 500-fold increase in binding potency observed upon sulfation of CCK-8, suggesting that the lysine appendage and the sulfated tyrosine in CCK-8, both key structural elements that impart high affinity for the CCK-A receptor, are interacting differently with the receptor. The amide-bearing tetrapeptides are full agonists relative to CCK-8 in stimulating pancreatic amylase release while being partial agonists in eliciting phosphoinositide (PI) hydrolysis. Both effects were blocked by selective CCK-A receptor antagonists.

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 2

IT 131448-82-3P 131448-83-4P 131448-84-5P 131448-85-6P 131448-86-7P
131448-87-8P 131448-88-9P 131448-89-0P 131448-90-3P 131448-91-4P
131448-92-5P 131448-93-6P 131448-94-7P 131448-95-8P 131448-97-0P
131448-98-1P 131448-99-2P 131449-00-8P 131449-01-9P 131449-02-0P
131449-03-1P 131449-05-3P 131449-06-4P 131449-07-5P 131449-08-6P
131449-10-0P 131449-11-1P 131449-15-5P 131449-18-8P 131449-19-9P
131449-21-3P 131449-22-4P 131449-23-5P 131449-24-6P 131449-36-0P
131449-38-2P 131449-39-3P 131449-40-6P 131449-41-7P
131449-47-3P 131449-49-5P 131449-50-8P 131449-63-3P
131449-68-8P 131450-20-9P 131450-22-1P 131469-93-7P 131469-95-9P
131470-01-4P 141397-91-3P 141397-92-4P 141397-93-5P 141397-94-6P
141397-96-8P 141397-98-0P 141397-99-1P 141407-52-5P 141407-53-6P
141411-08-7P 141411-09-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as selective CCK-A receptor agonist)

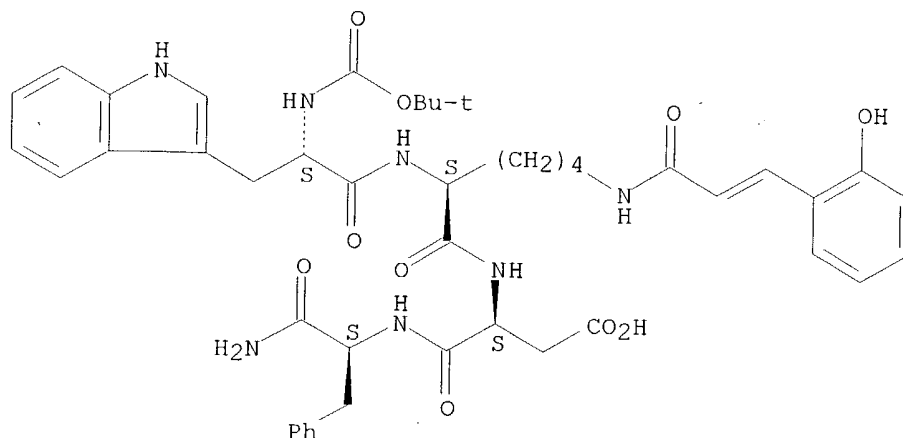
IT **131449-47-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as selective CCK-A receptor agonist)

RN 131449-47-3 HCA

CN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-tryptophyl-N6-[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]-L-lysyl-L- α -aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



QD 380.M3

L57 ANSWER 12 OF 15 HCA COPYRIGHT 2004 ACS on STN

113:59902 Synthesis and properties of polyamides having anti head-to-head umbelliferone dimer as a component. Saigo, Kazuhiko; Nakamura, Masataka; Suzuki, Yohko; Fang, Ian; Hasegawa, Masaki (Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan). Macromolecules, 23(16), 3722-9 (English) 1990. CODEN: MAMOBX. ISSN: 0024-9297.

AB anti Head-to-head umbelliferone dimer (I) was prepared from anti head-to-head 7-acetoxycoumarin dimer. The ring-opening polyaddn. reaction of I with diamines in an aprotic polar solvent was carried out, and the properties of the resulting polyamides were investigated. I reacted successfully with aliphatic and **aromatic** diamines to give the corresponding high-mol.-weight polyamides. Upon photoirradn., the cyclobutanes in the main chain of the polyamides were preferentially cleaved in an asym. manner to give fumaramide (or maleamide) units. In contrast, in an alkaline solution, the cyclobutanes in the polyamide were

cleaved only in a sym. manner to give low-mol.-weight products, accompanying the isomerization of the configuration of the substituents on the cyclobutanes. These reactions in alkaline medium are considered to occur through an intermediate of a quinoid enolate structure.

CC 35-3 (Chemistry of Synthetic High Polymers)

IT 93-35-6P **128327-78-6P** 128327-79-7P 128440-13-1P
128441-96-3P

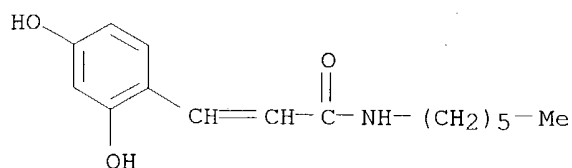
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by alkaline hydrolysis of amine-umbelliferone dimer reaction products)

IT **128327-78-6P**

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by alkaline hydrolysis of amine-umbelliferone dimer reaction products)

RN 128327-78-6 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-hexyl- (9CI) (CA INDEX NAME)



L57 ANSWER 13 OF 15 HCA COPYRIGHT 2004 ACS on STN

96:100319 Separation of some metabolically important **aromatic** N-acylamino acids of the benzoyl and cinnamoyl series by thin-layer, gas-liquid and high-performance liquid chromatography. Van Sumere, Christiaan F.; Van de Castele, Karel; Hanselaer, Rene; Martens, Marc; Geiger, Hans; Van Rompaey, Luc (Lab. Plant Biochem., Rijksuniv. Gent, Ghent, 9000, Belg.). Journal of Chromatography, 234(1), 141-55 (English) 1982. CODEN: JOCRAM. ISSN: 0021-9673.

AB The sepns. of 30 different N-acyl amino acids and peptides from the benzoyl and cinnamoyl series were studied by TLC, gas chromatog. (GC), and high-performance liquid chromatog. (HPLC). TLC sepns. on 3 different layers and with 4 different solvent systems are described. GC sepns. of the trimethylsilyl derivs. of some of the compds. were carried out on a glass column packed with Chromosorb W AW DMCS (80-100 mesh) coated with 1.5% SE-30 + 1.5% SE-52 and using a temperature program. HPLC sepns. on a reversed-phase column (LiChrosorb RP-18, 10 μ m) used a combination of isocratic and linear gradient elution [solvent A, H₂O-HCO₂H (95:5); solvent B, MeOH; 35°]. The few compds. which could not be separated by the latter system were separated on a 2nd column (LiChrosorb Si 60, 7 μ m) by means of a combination of isocratic and linear gradient elution [solvent A, CH₂Cl₂-cyclohexane-HCO₂H (55:45:2); solvent B, MeOH; 30°]. These methods can easily be combined and allow the separation of N-acyl amino acids and N-acyl peptides from biol. fluids, exts., and partial hydrolyzates from phenolic acid-containing plant protein.

CC 9-3 (Biochemical Methods)

IT 487-54-7 495-69-2 1212-04-0 1220-05-9 1637-75-8 2482-25-9
10003-42-6 16533-60-1 16534-24-0 40747-82-8 62098-75-3
62098-77-5 70120-43-3 70702-59-9 80922-82-3 80922-83-4
80922-84-5 80922-85-6 80922-86-7 80922-87-8 80922-88-9
80922-89-0 80922-90-3 **80922-91-4** 80922-92-5 80922-93-6
80922-94-7 80922-95-8 80952-39-2 80952-40-5

RL: ANT (Analyte); ANST (Analytical study)

(determination of, by gas chromatog. and high-performance liquid chromatog.

and

TLC)

IT **80922-91-4**

RL: ANT (Analyte); ANST (Analytical study)

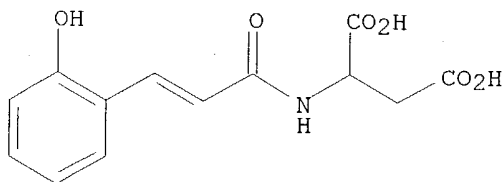
(determination of, by gas chromatog. and high-performance liquid chromatog.

and

TLC)

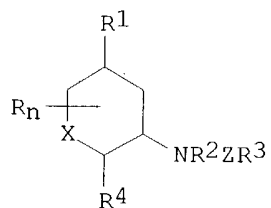
RN 80922-91-4 HCA

CN Aspartic acid, N-[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

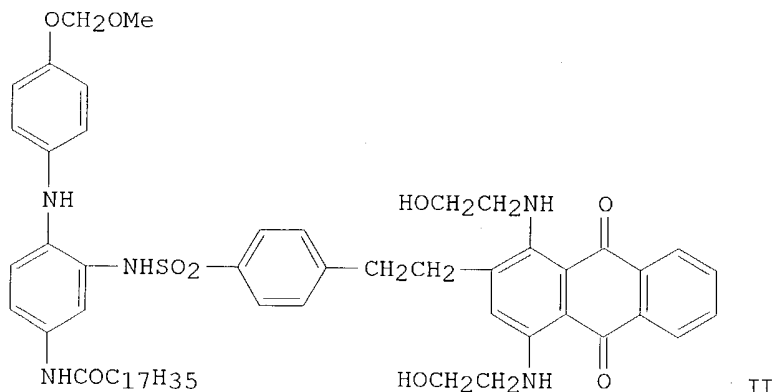


L57 ANSWER 14 OF 15 HCA COPYRIGHT 2004 ACS on STN
 90:123080 Anthraquinone compounds useful in photographic processes. Bloom,
 Stanley M. (Polaroid Corp., USA). U.S. US 4110355 19780829, 21 pp.
 (English). CODEN: USXXAM. APPLICATION: US 1973-363354 19730523.

GI



I



II

AB Color developers (I, R = anchoring substituent rendering I nondiffusible;
 R1 = HO or amino derivative; R2 = H or alkyl; R3 = anthraquinone dye residue;
 R4 = H or substituent replaceable by an oxidized **aromatic** amino
 color developer in elimination-coupling reactions chosen from Cl, Br,
 CO2H, SO3H, alkoxy, or hydroxyalkyl; X = atoms necessary to complete a
 benzene or naphthalene residue, n = 0 or 1; n = 0 where R1 = in a
 secondary or tertiary amino group comprising an anchoring group) were
 prepared and were useful in photog. emulsions for color photog. Azo dyes
 (I, R3 = azo chromophore) were also prepared and used. Thus, II
 [69477-78-7] was prepared by conventional methods.

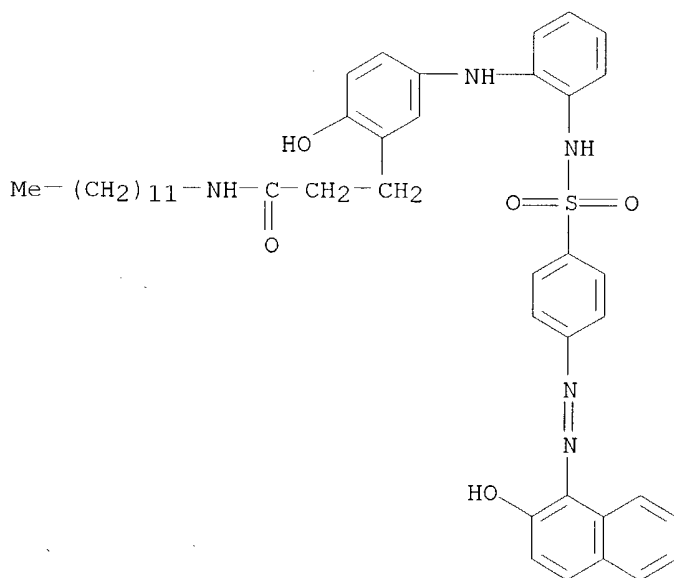
IC C09B001-50

NCL 260372000

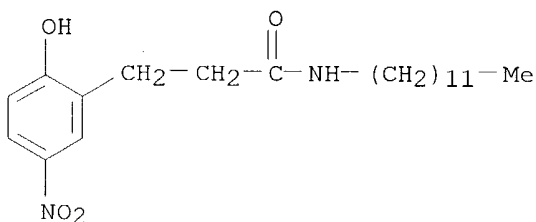
CC 40-12 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

IT 24355-40-6 **24355-47-3**

RL: USES (Uses)
 (color developer, for photog., preparation of)
 IT **24355-41-7** 24355-51-9 69477-74-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (methylation of)
 IT 24355-52-0P **24355-58-6P** 69477-78-7P
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of)
 IT **24355-47-3**
 RL: USES (Uses)
 (color developer, for photog., preparation of)
 RN 24355-47-3 HCA
 CN Benzenepropanamide, N-dodecyl-2-hydroxy-5-[[2-[[[4-[(2-hydroxy-1-naphthalenyl)azo]phenyl]sulfonyl]amino]phenyl]amino]- (9CI) (CA INDEX NAME)



IT **24355-41-7**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (methylation of)
 RN 24355-41-7 HCA
 CN Benzenepropanamide, N-dodecyl-2-hydroxy-5-nitro- (9CI) (CA INDEX NAME)

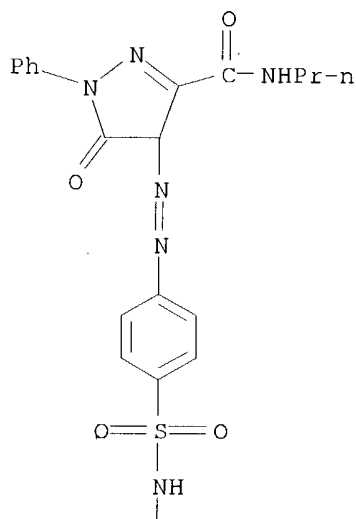


A suggested bond

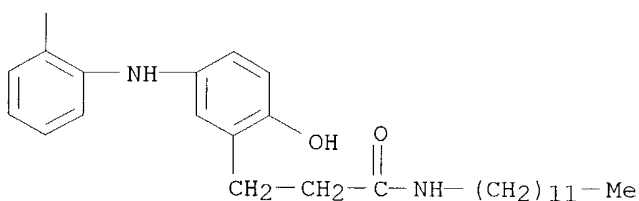
IT **24355-58-6P**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of)
 RN 24355-58-6 HCA

CN 1H-Pyrazole-3-carboxamide, 4-[[4-[[[2-[[3-[3-(dodecylamino)-3-oxopropyl]-4-hydroxyphenyl]amino]phenyl]amino]sulfonyl]phenyl]azo]-4,5-dihydro-5-oxo-1-phenyl-N-propyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L57 ANSWER 15 OF 15 HCA COPYRIGHT 2004 ACS on STN

72:127282 Reducing agents providing color image stabilization. Bloom, Stanley M.; Huyffer, Paul S. (Polaroid Corp.). U.S. US 3482971 19691209, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 1967-655324 19670724.

GI For diagram(s), see printed CA Issue.

AB Immobile reducing agents react with the oxidized developer and form a new immobile heterocyclic ring which prevents a color change in pos. dye-diffusion transfer image systems. The preferred reducing agents are I and II and may be synthesized by reacting an acid salt with the 3-amino substituent of the **aromatic** ring. E.g., a photosensitive element for example was prepared by coating on a cellulose acetate support a gelatin layer containing colloidal Ag, Ag-precipitating agent (136 mg/ft²), and the

color-providing composition III (136 mg/ft²) and overcoating with gelatin and I (each 136 mg/ft²) and a layer of Ag iodobromide emulsion. After light exposure and a 2-min development with a solution containing H₂O 100 ml, (hydroxyethyl)cellulose 3.9, NaOH 4.0, Na₂S₂O₃·5H₂O 2.0, Na₂SO₃ 2.0, and Metol 1.6 g by spreading it between the exposed element and a superposed dyeable sheet at a 0.0026 in. gap, a pos. dye-transfer image was obtained.

IC G03C

NCL 096003000

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)

IT 28374-02-9 28374-06-3

RL: USES (Uses)

(photographic dye diffusion-transfer emulsions containing)

IT 24355-41-7P 24355-42-8P 24355-43-9P 24355-44-0P

24355-45-1P 28020-15-7P 28374-03-0P 28374-04-1P 28374-05-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

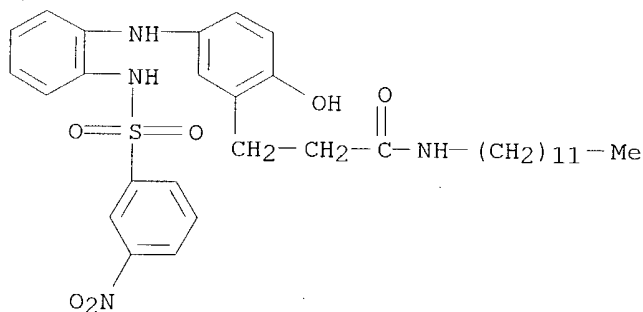
IT 28374-02-9

RL: USES (Uses)

(photographic dye diffusion-transfer emulsions containing)

RN 28374-02-9 HCA

CN Hydrocinnamamide, N-dodecyl-2-hydroxy-5-[o-(p-nitrobenzenesulfonamido)anilino]- (8CI) (CA INDEX NAME)

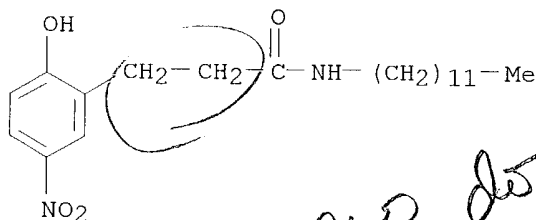


IT 24355-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24355-41-7 HCA

CN Benzenepropanamide, N-dodecyl-2-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



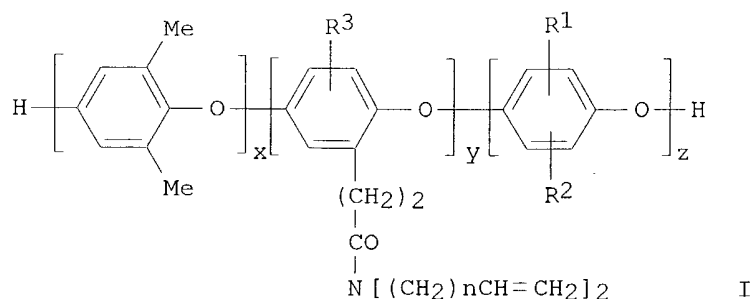
=> D 158 1-10 CBIB ABS HITSTR

L58 ANSWER 1 OF 47 HCA COPYRIGHT 2004 ACS on STN

140:5605 Polyphenylene ether copolymers having dialkenylamide groups and their

preparation and their compositions. Wang, Shin-Shin; Ma, Jie-Hwa; Yang, Jong-Lieh; Hsu, Kuo-Yuan; Liang, Li-Chung (Industrial Technology Research Institute, Taiwan). U.S. Pat. Appl. Publ. US 2003225220 A1 20031204, 10 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-308125 20021203. PRIORITY: TW 2002-91111095 20020524.

GI



AB The polyphenylene ether copolymer having di(C2-10 linear alkenylamide) group is represented a formula I ($x = 1-80\%$; $y = 1-10\%$; $z = 1-40\%$; $x + y + z = 100\%$, $n = 0-10$; $R1 = H$, C1-10 linear or branched alkyl; $R2 = H$, C1-10 linear or branched alkyl, C2-10 linear or branched alkenyl; and $R3 = H$, C2-10 linear or branched alkenyl). The resin composition having a low crosslinking temperature comprises the PPE copolymer and a free-radical initiator. Thus, 4.5 parts 2-allyl-6-methylphenol-N,N-diallyl-3-(2-hydroxyphenyl) propionamide-2,6-dimethylphenol copolymer was mixed with triallyl isocyanurate 1.15 and 2,5-dimethyl-2,5-di-tert-butylperoxyhexane 0.175 parts, press at 200° for 60 min, to give a sheet showing dissipation factor <2.8 , and Tg 188° .

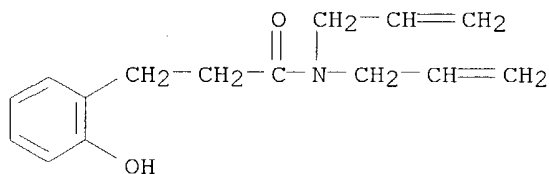
IT 627102-64-1P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(monomer; preparation of polyphenylene ether copolymers having dialkenylamide groups for low-temperature curable compns.)

RN 627102-64-1 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-di-2-propenyl- (9CI) (CA INDEX NAME)



IT 627102-65-2P 627102-67-4P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation of polyphenylene ether copolymers having dialkenylamide groups for low-temperature curable compns.)

RN 627102-65-2 HCA

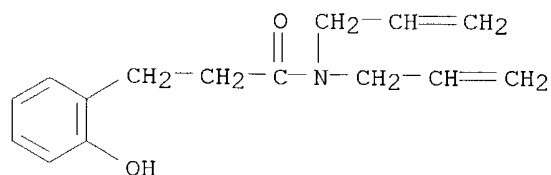
CN Benzenepropanamide, 2-hydroxy-N,N-di-2-propenyl-, polymer with

2,6-dimethylphenol and 2-methyl-6-(2-propenyl)phenol (9CI) (CA INDEX NAME)

CM 1

CRN 627102-64-1

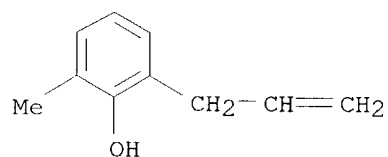
CMF C15 H19 N O2



CM 2

CRN 3354-58-3

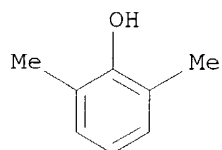
CMF C10 H12 O



CM 3

CRN 576-26-1

CMF C8 H10 O



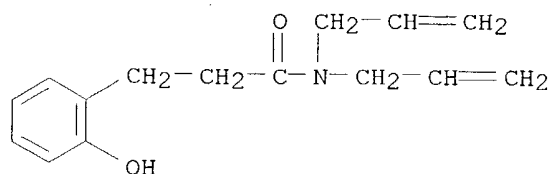
RN 627102-67-4 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-di-2-propenyl-, polymer with 2,6-dimethylphenol and 2-methyl-6-(1-methylethyl)phenol (9CI) (CA INDEX NAME)

CM 1

CRN 627102-64-1

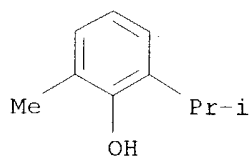
CMF C15 H19 N O2



CM 2

CRN 3228-04-4

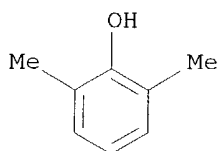
CMF C10 H14 O



CM 3

CRN 576-26-1

CMF C8 H10 O



IT 627102-68-5P 627102-70-9P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of polyphenylene ether copolymers having dialkenylamide groups for low-temperature curable compns.)

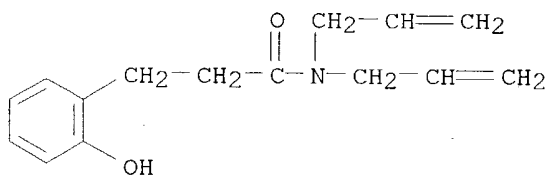
RN 627102-68-5 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-di-2-propenyl-, polymer with 2,6-dimethylphenol, 2-methyl-6-(2-propenyl)phenol and 1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (9CI) (CA INDEX NAME)

CM 1

CRN 627102-64-1

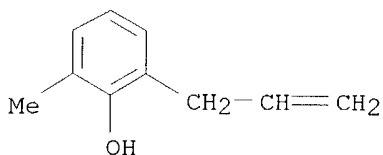
CMF C15 H19 N O2



CM 2

CRN 3354-58-3

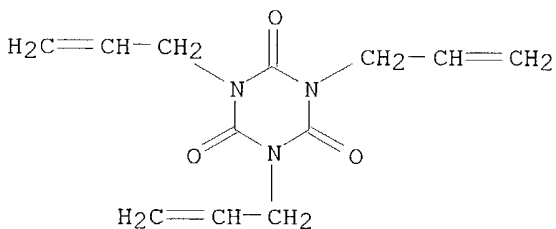
CMF C10 H12 O



CM 3

CRN 1025-15-6

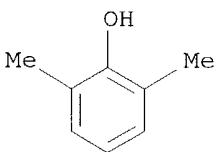
CMF C12 H15 N3 O3



CM 4

CRN 576-26-1

CMF C8 H10 O



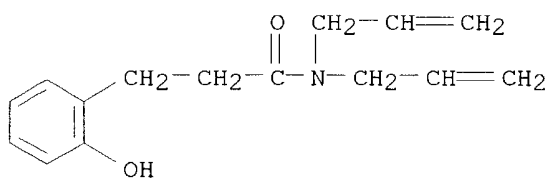
RN 627102-70-9 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-di-2-propenyl-, polymer with 2,6-dimethylphenol, 2-methyl-6-(1-methylethyl)phenol and 1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (9CI) (CA INDEX NAME)

CM 1

CRN 627102-64-1

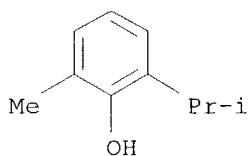
CMF C15 H19 N O2



CM 2

CRN 3228-04-4

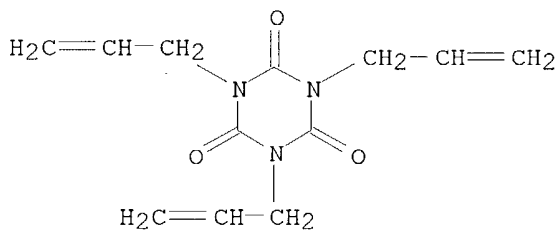
CMF C10 H14 O



CM 3

CRN 1025-15-6

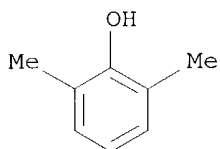
CMF C12 H15 N3 O3



CM 4

CRN 576-26-1

CMF C8 H10 O



L58 ANSWER 2 OF 47 HCA COPYRIGHT 2004 ACS on STN
 138:260196 A Modified Coumarinic Acid-Based Cyclic Prodrug of an Opioid
 Peptide: Its Enzymatic and Chemical Stability and Cell Permeation
 Characteristics. Ouyang, Hui; Tang, Fuxing; Siahaan, Teruna J.;
 Borchardt, Ronald T. (Department of Pharmaceutical Chemistry, The

University of Kansas, Lawrence, KS, 66049, USA). Pharmaceutical Research, 19(6), 794-801 (English) 2002. CODEN: PHREEB. ISSN: 0724-8741.

Publisher: Kluwer Academic/Plenum Publishers.

- AB This study was to evaluate the chemical/enzymic stability and the cell permeation characteristics of the modified coumarinic acid-based cyclic prodrug (I, c[Tyr-D-Ala-Gly-Phe-D-Leu-OCH₂OC₆H₄-o-CH:CH₆) of DADLE (H-Tyr-D-Ala-Gly-Phe-D-Leu-OH), which has an aldehyde equivalent (oxymethyl) inserted between the phenolic group of the promoiety and the carboxylic acid group of the peptide. The rates of the chemical/enzymic conversion of I to DADLE were measured by HPLC. The cellular permeation characteristics of DADLE and its oxymethyl-modified prodrug 2 were measured by HPLC using Caco-2 cells, wild type Madin-Darby Canine Kidney cells (MDCK-WT), MDCK cells transfected with human MDR1 gene (MDCK-MDR1), and MDCK cells transfected with human MRP2 gene (MDCK-MRP2) grown onto microporous membranes. I degraded chemical to DADLE in a pH-dependent manner, i.e., rates of conversion increased with increasing pH. I degraded rapidly in rat plasma (t_{1/2} = 39 min) and rat liver homogenate (t_{1/2} = 59.2 min), but much slower in Caco-2 cell homogenate (t_{1/2} = 678.7 min) and human plasma (t_{1/2} = 264.3 min). In all four cell lines used for transport studies, the flux rates of I in the basolateral (BL)-to-apical (AP) direction (Papp BL-to-AP) were significantly greater than the flux rates in the AP-to-BL direction (Papp AP-to-BL). The Papp BL-to-AP /Papp AP-to-BL ratios were >116, 35.1, 21.2, and 12.6 in Caco-2, MDCK-MDR1, MDCK-MRP2, and MDCK-WT cells, resp. The efflux of the modified prodrug could be inhibited by GF120918 (an inhibitor for P-gp) and cyclosporin A (an inhibitor for P-gp and MRP2). I of DADLE could be converted to DADLE in both chemical and enzymic media. However, the prodrug was a good substrate for both P-gp and MRP2 suggesting that its permeation across intestinal mucosa and blood-brain barrier would be significantly restricted.

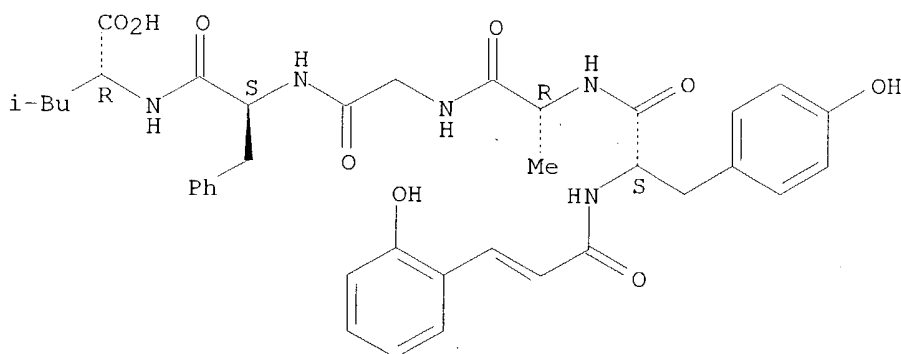
IT 502561-12-8

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(enzymic and chemical stability and cell permeation of a modified coumarinic acid-based cyclic prodrug of an opioid peptide)

RN 502561-12-8 HCA

CN D-Leucine, N-[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]-L-tyrosyl-D-alanylglycyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L58 ANSWER 3 OF 47 HCA COPYRIGHT 2004 ACS on STN

138:249902 Fungal glyoxal oxidases and genes/cDNAs, their use in fungicide screening, and methods of enhancing resistance of plants to phytopathogenic fungi. Aichinger, Christian; Schreier, Peter; Leuthner, Brigitta; Adamczewski, Martin; Hillebrand, Stefan; Kuck, Karl-Heinz; Van Kan, Johannes Arnoldus Laurentius; Visser, Jaap; Stefanato, Francesca Maria; Kahmann, Regine; Boelker, Michael (Bayer CropScience AG, Germany). Eur. Pat. Appl. EP 1293562 A1 20030319, 97 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK. (German). CODEN: EPXXDW. APPLICATION: EP 2002-19172 20020902. PRIORITY: DE 2001-10145095 20010913; DE 2001-10159375 20011204; DE 2002-10221725 20020516.

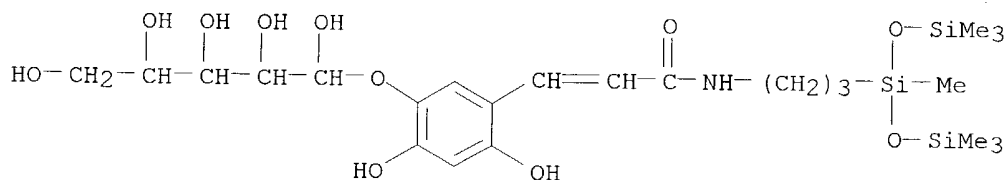
AB Disclosed are *Ustilago maydis* and *Botrytis cinerea* glyoxal oxidases as well as cDNAs and genes encoding these enzymes. The enzymes, or cells producing these enzymes, may be used to screen for fungicides. Phytopathogenic fungi in which the glyoxal oxidase genes have been knocked out may be used to stimulate pathogen resistance in plants. Thus, *U. maydis* glol gene knockouts and *B. cinerea* glyoxl gene knockouts were prepared. These recombinant fungi were not pathogenic to tomatoes and apples. *U. maydis* transformants overexpressing the glol gene were used to identify potential fungicidal compds.

IT 501424-88-0

RL: BSU (Biological study, unclassified); BIOL (Biological study) (glyoxal oxidase inhibitor; fungal glyoxal oxidases and genes/cDNAs, their use in fungicide screening, and methods of enhancing resistance of plants to phytopathogenic fungi)

RN 501424-88-0 HCA

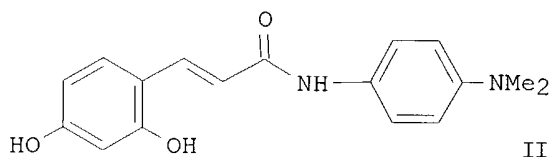
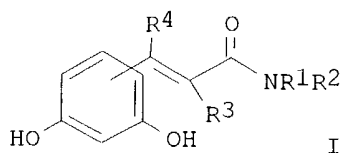
CN Pentose, 2,4-dihydroxy-5-[3-oxo-3-[[3-[1,3,3,3-tetramethyl-1-[(trimethylsilyl)oxy]disiloxanyl]propyl]amino]-1-propenyl]phenyl hemiacetal (9CI) (CA INDEX NAME)



L58 ANSWER 4 OF 47 HCA COPYRIGHT 2004 ACS on STN

135:288586 Preparation of (dihydroxyphenyl)acrylamide derivatives and compositions containing coloring agents. (Wella AG, Germany). Ger. Gebrauchsmusterschrift DE 20110355 U1 20011004, 52 pp. (German). CODEN: GGXXFR. APPLICATION: DE 2001-20110355 20010622.

GI



AB (m-dihydroxyphenyl)acrylamide derivs. I [R1, R2 = H, C1-2-alkoxy, C1-6-alkyl, C3-6-alkenyl, C2-4-hydroxyalkyl, C3-4-dihydroxyalkyl, C2-4-aminoalkyl, C2-4-dimethylaminoalkyl, C2-4-acetylaminoalkyl, C2-4-methoxyalkyl, C2-4-ethoxyalkyl, C1-4-cyanoalkyl, C1-4-carboxyalkyl, C1-4-aminocarbonylalkyl, pyridylmethyl, furfuryl, hydrogenated furfuryl, substituted pyridyl, CHR5CHR6R7, (un)substituted Ph, aminopyrazolyl; R1R2N = (un)substituted piperidine, morpholine, the formulpiperazine, pyrrolidine; R3, R4 = H, C1-4-alkyl; R5 = H, CO2H, CONH2; R6, R7 = H, OH, CONH2, CH2SMe, PH, hydroxyphenyl, morpholinyl, oxopyrrolidinyl, imidazolyl] or its physiol. compatible, water-soluble salts are claimed. Thus, 3-(2,4-dihydroxyphenyl)-N-[4-(dimethylamino)phenyl]acrylamide hydrochloride (II·HCl), was prepared from 2,4-(HO)2C6H4CHO, via hydroxyl group protection, Wittig with (MeO2C)CH:PPh3, saponification, amidation with 4-(Me2N)C6H4NH2 and deprotection. I were used in the preparation of hair dye formulations and their color tints noted.

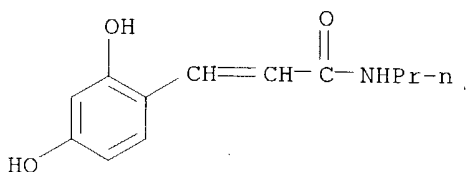
IT 364326-44-3P 364326-46-5P 364326-49-8P
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 364326-62-5P 364326-70-5P 364326-71-6P
 364326-87-4P 364326-88-5P 364327-45-7P
 364327-47-9P 364327-50-4P 364327-54-8P
 364327-59-3P 364327-61-7P 364327-63-9P
 364327-65-1P 364327-72-0P 364327-73-1P
 364327-91-3P 364327-92-4P 364328-19-8P

RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(oxidative hair dye component; preparation of (dihydroxyphenyl)acrylamide derivs. and compns. containing coloring agents)

RN 364326-44-3 HCA

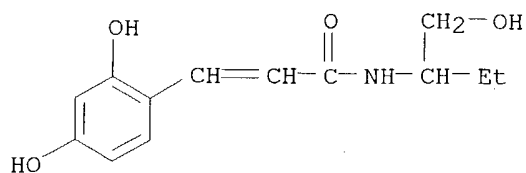
CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-propyl- (9CI) (CA INDEX NAME)



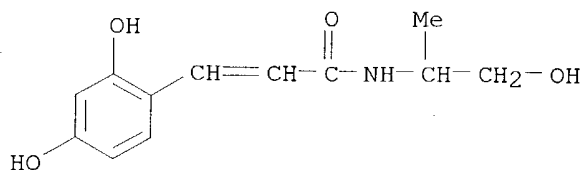
RN 364326-46-5 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-[1-(hydroxymethyl)propyl]- (9CI)

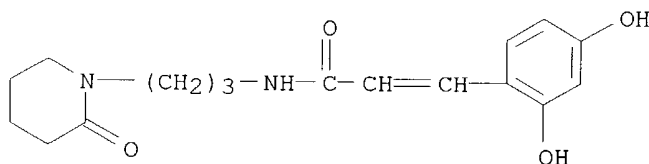
(CA INDEX NAME)



RN 364326-49-8 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-(2-hydroxy-1-methylethyl)- (9CI)
(CA INDEX NAME)

RN 364326-57-8 HCA

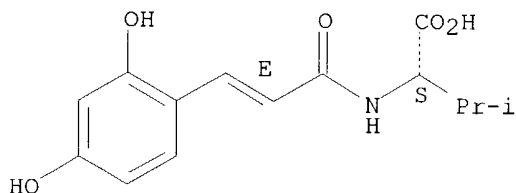
CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-[3-(2-oxo-1-piperidinyl)propyl]-
(9CI) (CA INDEX NAME)

RN 364326-58-9 HCA

CN L-Valine, N-[(2E)-3-(2,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA
INDEX NAME)

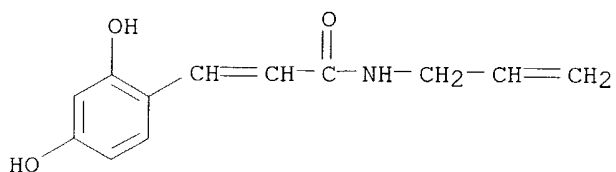
Absolute stereochemistry.

Double bond geometry as shown.

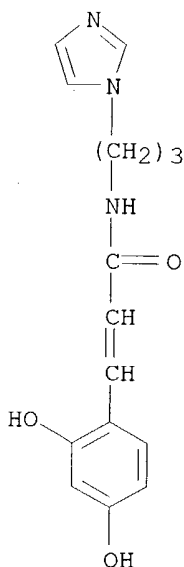


RN 364326-60-3 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-2-propenyl- (9CI) (CA INDEX
NAME)



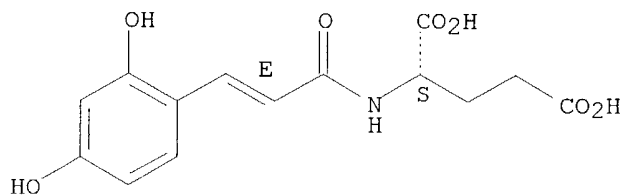
RN 364326-62-5 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-[3-(1H-imidazol-1-yl)propyl]-
(9CI) (CA INDEX NAME)

RN 364326-70-5 HCA

CN L-Glutamic acid, N-[(2E)-3-(2,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI)
(CA INDEX NAME)

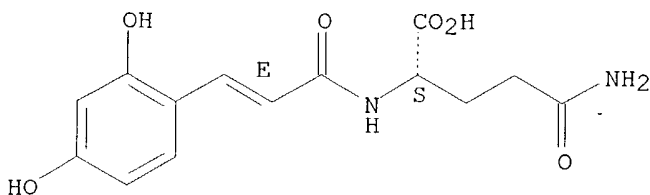
Absolute stereochemistry.
Double bond geometry as shown.



RN 364326-71-6 HCA

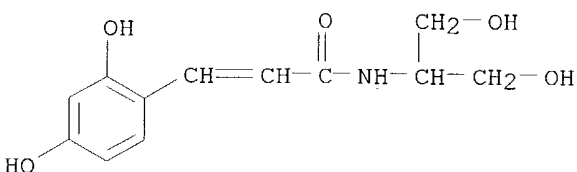
CN L-Glutamine, N2-[(2E)-3-(2,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 364326-87-4 HCA

CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-[2-hydroxy-1-(hydroxymethyl)ethyl]- (9CI) (CA INDEX NAME)

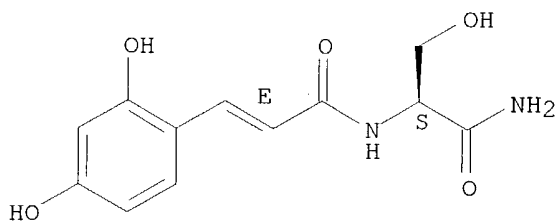


RN 364326-88-5 HCA

CN 2-Propenamide, N-[(1S)-2-amino-1-(hydroxymethyl)-2-oxoethyl]-3-(2,4-dihydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

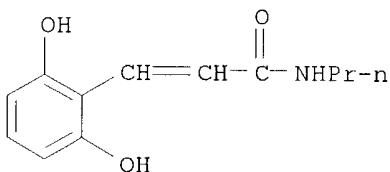
Absolute stereochemistry.

Double bond geometry as shown.



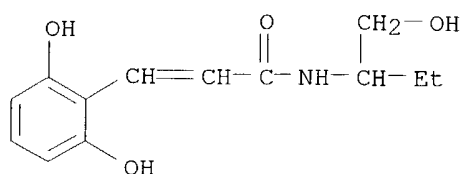
RN 364327-45-7 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-propyl- (9CI) (CA INDEX NAME)

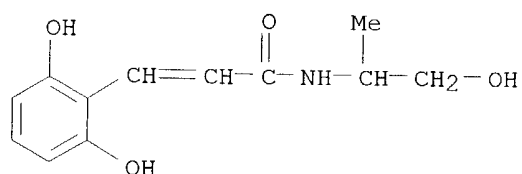


RN 364327-47-9 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-[1-(hydroxymethyl)propyl]- (9CI) (CA INDEX NAME)

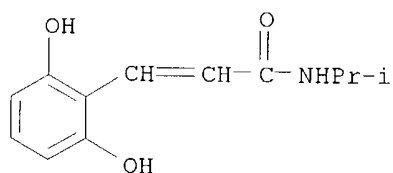


RN 364327-50-4 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-(2-hydroxy-1-methylethyl)- (9CI)
(CA INDEX NAME)

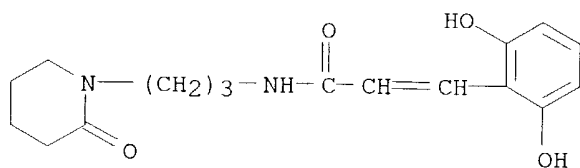
RN 364327-54-8 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 364327-59-3 HCA

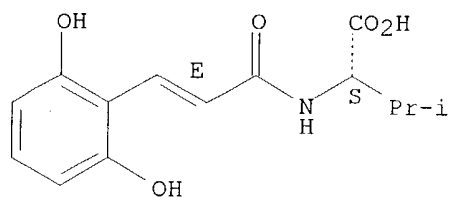
CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-[3-(2-oxo-1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)



RN 364327-61-7 HCA

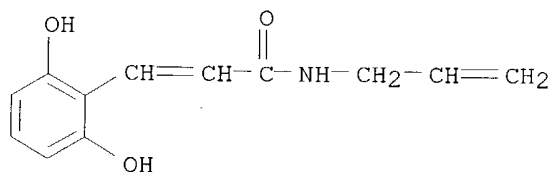
CN L-Valine, N-[(2E)-3-(2,6-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



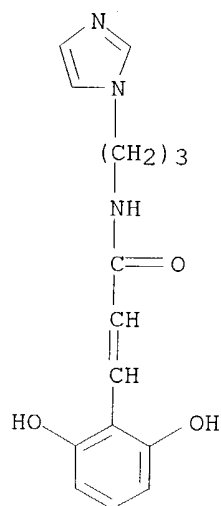
RN 364327-63-9 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



RN 364327-65-1 HCA

CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-[3-(1H-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

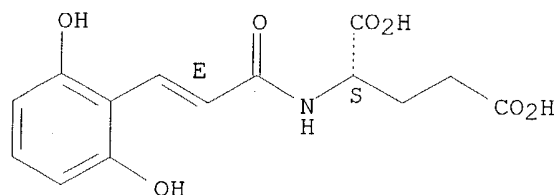


RN 364327-72-0 HCA

CN L-Glutamic acid, N-[(2E)-3-(2,6-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

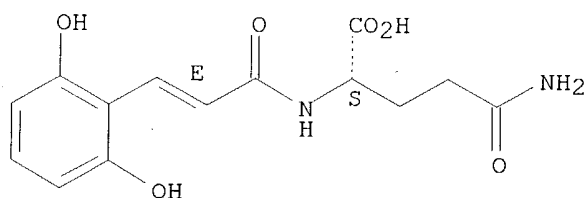
Double bond geometry as shown.



RN 364327-73-1 HCA

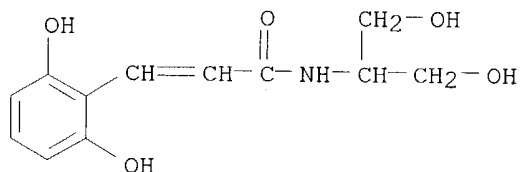
CN L-Glutamine, N2-[(2E)-3-(2,6-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 364327-91-3 HCA

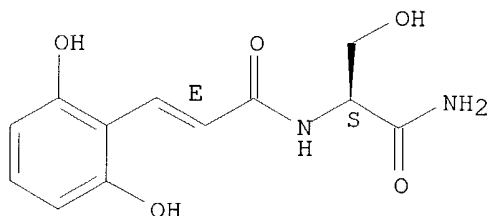
CN 2-Propenamide, 3-(2,6-dihydroxyphenyl)-N-[2-hydroxy-1-(hydroxymethyl)ethyl]- (9CI) (CA INDEX NAME)



RN 364327-92-4 HCA

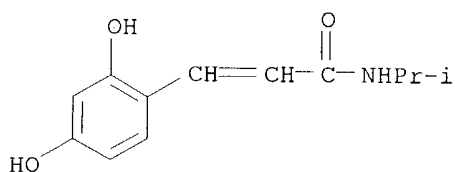
CN 2-Propenamide, N-[(1S)-2-amino-1-(hydroxymethyl)-2-oxoethyl]-3-(2,6-dihydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 364328-19-8 HCA

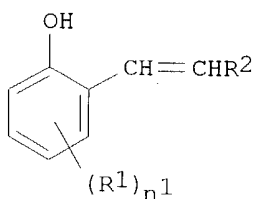
CN 2-Propenamide, 3-(2,4-dihydroxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



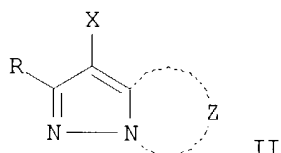
L58 ANSWER 5 OF 47 HCA COPYRIGHT 2004 ACS on STN

133:200808 Silver halide color photographic material with improved light-resistant magenta image. Ishii, Fumio (Konica Co., Japan). Jpn. Kokai Tokkyo Koho JP 2000235246 A2 20000829, 35 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-35812 19990215.

GI



I



II

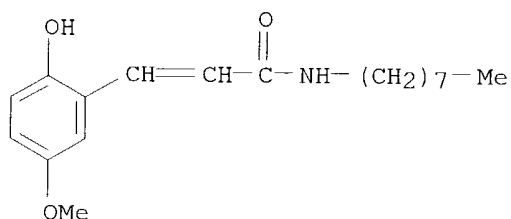
AB The title photog. material contains an image stabilizer represented by the general formula I (R_1 , R_2 = substituent; n_1 = 1-4) and a magenta coupler represented by the general formula II (R = H, substituent; X = H, group capable of cleaving upon reaction with developing agent oxide; Z = atoms for forming N-containing heterocycle ring) in a photog. layer.

IT 289623-40-1

RL: DEV (Device component use); USES (Uses)
(stabilizer in Ag halide color photog. material with improved light-resistant magenta image)

RN 289623-40-1 HCA

CN 2-Propenamide, 3-(2-hydroxy-5-methoxyphenyl)-N-octyl- (9CI) (CA INDEX NAME)



L58 ANSWER 6 OF 47 HCA COPYRIGHT 2004 ACS on STN

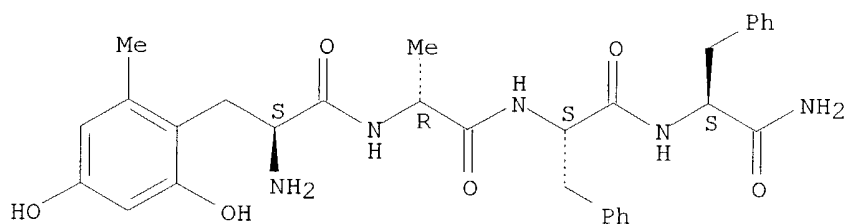
133:12871 Opioid peptide analogs containing 2'-hydroxy,6'-methyltyrosine in place of Tyr1 display greatly enhanced δ antagonist potency but unchanged μ agonist potency. Berezowska, Irena; Lemieux, Carole; Nguyen, Thi M. -D.; Chung, Nga N.; Schiller, Peter W. (Clinical Research Institute of Montreal, Montreal, QC, H2W 1R7, Can.). Peptides 1998,

Proceedings of the European Peptide Symposium, 25th, Budapest, Aug. 30-Sept. 4, 1998, Meeting Date 1998, 718-719. Editor(s): Bajusz, Sandor; Hudecz, Ferenc. Akademiai Kiado: Budapest, Hung. (English) 1999. CODEN: 68WKAY.

- AB The authors report the syntheses and in vitro opioid activity profiles of the Hmt1-analogs of the δ antagonists TIP (H-Tyr-Tic-Phe-OH) and TIPP (H-Tyr-Tic-Phe-Phe-OH) and of the μ agonists TAPP (H-Tyr-D-Ala-Phe-Phe-NH₂) and DALDA (H-Tyr-D-Arg-Phe-Lys-NH₂). In vitro opioid activities of the compds. were determined in the μ -receptor-representative guinea pig ileum assay and in the δ receptor-representative mouse vas deferens (MVD) assay, and their μ and δ receptor affinities were measured in binding assays based on displacement of [3H]DAMGO and [3H]DSLET, resp., from rat brain membrane binding sites. The tripeptide H-Hmt-Tic-Phe-OH was an about 15 times more potent δ antagonist against the δ agonist DPDPE than its parent TIP, showing δ antagonist potency (MVD) and δ receptor binding affinity in the subnanomolar range. Furthermore, this compound showed greatly improved δ receptor selectivity as compared to TIP. The Hmt1-analog of the tetrapeptide TIPP, H-Hmt-Tic-Phe-Phe-OH, displayed very high δ antagonist potency in the MVD assay, comparable to that of H-Dmt-Tic-Phe-Phe-OH. In the binding assays, it showed slightly higher δ receptor affinity than H-Dmt-Tic-Phe-Phe-OH and 20-fold higher δ selectivity. Thus, [Hmt1]TIPP ranks among the most potent and most specific δ opioid antagonists reported to date. Substitution of Hmt for Tyr1 in the μ agonist peptides TAPP and DALDA resulted in μ -agonist potencies comparable to those of their resp. parent peptides,. In conclusion, replacement of Tyr1 in opioid peptides with Hmt produced a potency increase in the case of the δ antagonists but not in the case of the μ agonists.

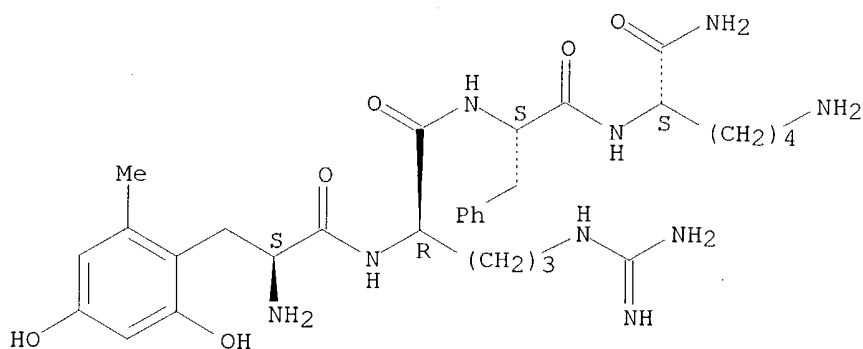
- IT 271795-38-1 271795-39-2
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(opioid peptide analogs δ antagonist and μ agonist activity in relation to structure)
RN 271795-38-1 HCA
CN L-Phenylalaninamide, 2-hydroxy-6-methyl-L-tyrosyl-D-alanyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- RN 271795-39-2 HCA
CN L-Lysinamide, 2-hydroxy-6-methyl-L-tyrosyl-D-arginyl-L-phenylalanyl- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L58 ANSWER 7 OF 47 HCA COPYRIGHT 2004 ACS on STN

132:151567 Preparation of arylamidoalkylcarboxylic acids and compositions for delivering active agents.. Gschneidner, David; Leone-Bay, Andrea; Wang, Eric; Errigo, Lynn; Kraft, Kelly; Moye-Sherman, Destardi; Ho, Koc-Kan; Press, Jeffrey Bruce; Wang, Nai Fang (Emisphere Technologies, Inc., USA). PCT Int. Appl. WO 2000007979 A2 20000217, 53 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US17974 19990806. PRIORITY: US 1998-95778 19980807; US 1998-98500 19980831; US 1998-108366 19981113; US 1999-119207 19990205.

AB 135 Title compds. are claimed. Thus, Me azeloyl chloride was added dropwise to 2-amino-p-cresol in aqueous NaOH at 0° to give a residue which was stirred with aqueous NaOH in THF to give 4-HO-5-MeC6H3NHCO(CH2)7CO2H. Title compds. at 100-300 mg/kg with parathyroid hormone at 25-200 µg orally or intracolonicly in rats gave peak serum parathyroid hormone levels of 5-1459.71 pg/mL.

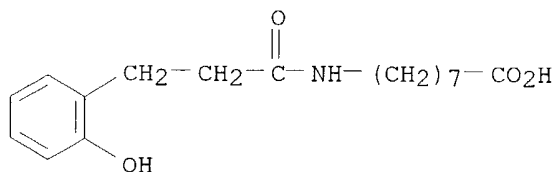
IT 257951-75-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylamidoalkylcarboxylic acids and compns. for delivering active agents)

RN 257951-75-0 HCA

CN Octanoic acid, 8-[[3-(2-hydroxyphenyl)-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 8 OF 47 HCA COPYRIGHT 2004 ACS on STN

131:222591 Complexation of Metal Ions with Amphiphilic O,O'-

Dihydroxyazobenzene Derivatives at the Air/Water Interface. Hwang, Mi-Ja;

Jeung, Chul-Seung; Suh, Junghun; Kim, Kwan (Department of Chemistry and Center for Molecular Catalysis, Seoul National University, Seoul, 151-742, S. Korea). Journal of Colloid and Interface Science, 216(1), 96-105 (English) 1999. CODEN: JCISA5. ISSN: 0021-9797. Publisher: Academic Press.

- AB The effect of metal salts (FeCl₃, FeCl₂, CuCl₂, CoCl₂, and [Co(NH₃)₅Cl]Cl₂) on the surface pressure-area isotherm of an O,O'-dihydroxyazobenzene-containing amphiphile was studied. The isotherm of the amphiphile was little affected in the presence of CuCl₂ and [Co(NH₃)₅Cl]Cl₂, but the isotherm was greatly affected by the presence of FeCl₃, FeCl₂, and CoCl₂, implying the formation of certain complexes at the air/H₂O interface. In the presence of salts in the H₂O subphase, Y-type Langmuir-Blodgett (LB) multilayers could be readily assembled on the arachidic acid precoated solid substrates. From UV/visible and ATR-IR spectroscopy, the coordinative polymerization of the azobenzene moieties was evidenced to occur when the Fe³⁺, Fe²⁺, Cu²⁺, and Co²⁺ ions were present in the H₂O subphase. The long axis of the azobenzene moiety seemed in all LB films to assume a nearly perpendicular orientation with respect to the solid substrate, but the orientation of the C:O bond appeared obviously different between the films prepared in the presence of FeCl₃ and CuCl₂. The IR spectral data indicated further that the alkyl chains in the LB film prepared in the presence of CuCl₂ assumed a more close-packed structure than those prepared in the presence of FeCl₃, along with an orientation 10° more tilted in the former than in the latter with respect to the surface normal. (c) 1999 Academic Press.

IT 243117-61-5 243117-62-6

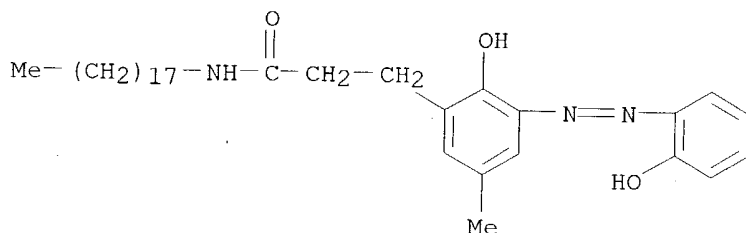
RL: RCT (Reactant); RACT (Reactant or reagent)

(effect of metal salts on surface pressure-area isotherm of

O,O'-dihydroxyazobenzene-containing amphiphile at air/water interface)

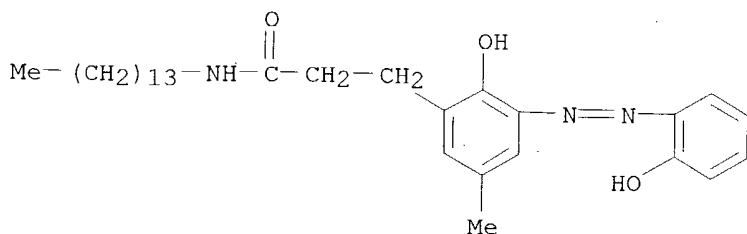
RN 243117-61-5 HCA

CN Benzenepropanamide, 2-hydroxy-3-[(2-hydroxyphenyl)azo]-5-methyl-N-octadecyl- (9CI) (CA INDEX NAME)



RN 243117-62-6 HCA

CN Benzenepropanamide, 2-hydroxy-3-[(2-hydroxyphenyl)azo]-5-methyl-N-tetradecyl- (9CI) (CA INDEX NAME)



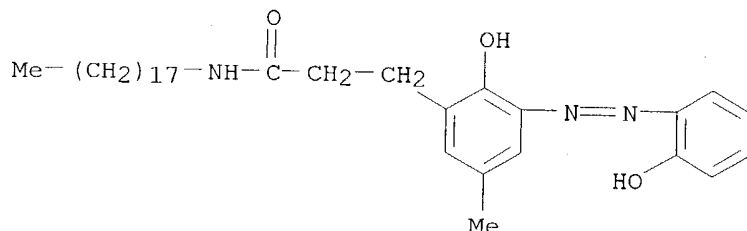
IT 243117-61-5D, Langmuir-Blodgett films containing iron or copper ions

243117-62-6D, Langmuir-Blodgett films containing iron or copper ions
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation and effect of metal salt on surface pressure-area isotherm at air/water interface)

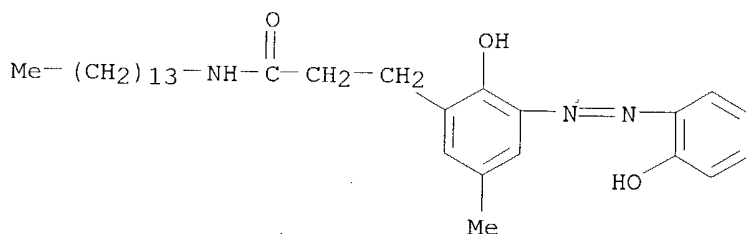
RN 243117-61-5 HCA

CN Benzenepropanamide, 2-hydroxy-3-[(2-hydroxyphenyl)azo]-5-methyl-N-octadecyl- (9CI) (CA INDEX NAME)



RN 243117-62-6 HCA

CN Benzenepropanamide, 2-hydroxy-3-[(2-hydroxyphenyl)azo]-5-methyl-N-tetradecyl- (9CI) (CA INDEX NAME)



L58 ANSWER 9 OF 47 HCA COPYRIGHT 2004 ACS on STN

130:337902 Two new improved approaches to the synthesis of coumarin-based prodrugs. Zheng, Ailian; Wang, Wei; Zhang, Huijuan; Wang, Binghe (Department of Chemistry, North Carolina State University, Raleigh, NC, 26795-8204, USA). Tetrahedron, 55(14), 4237-4254 (English) 1999. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier Science Ltd..

AB The development of a coumarin-based, esterase-sensitive prodrug system for the preparation of prodrugs of amines, peptides, and peptidomimetics was recently reported. Biol. evaluations including animal studies have demonstrated the clin. potential of this prodrug system. However, the original synthetic method used required a long sequence of reactions with a relatively low overall yield. Two new approaches to the synthesis of these coumarin-based prodrugs are now described. The first approach is a photochem. approach taking advantage of the photoisomerization of cinnamic acid and its derivs. The second approach is through the catalytic hydrogenation of a triple bond for the generation of the cis double bond in the coumarinic acid moiety. Both approaches allow for the synthesis of these prodrugs in fewer steps with much improved overall yield.

IT **190366-77-9P**

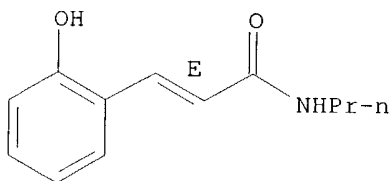
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of coumarinic acid prodrugs for peptidomimetics)

RN 190366-77-9 HCA

CN 2-Propenamide, 3-(2-hydroxyphenyl)-N-propyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L58 ANSWER 10 OF 47 HCA COPYRIGHT 2004 ACS on STN

130:222823 Parallel synthesis of 2-alkoxy- and 2-acyloxyphenylpropyl amides and amines using dihydrocoumarins as versatile synthons. Application of a novel resin quench-capture method. Bussolari, Jacqueline C.; Rehborn, Diana C.; Combs, Donald W. (The R.W. Johnson Pharmaceutical Research Institute, Drug Discovery, Raritan, NJ, 08869, USA). Tetrahedron Letters, 40(7), 1241-1244 (English) 1999. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd.,

AB A solution phase synthesis for the preparation of libraries of 2-substituted phenylpropyl amines and amides was accomplished using dihydrocoumarins as a useful synthon in parallel synthesis. Resin quench methods were utilized in the purifications of the amides and a resin quench-capture method was utilized in metallo-organic redns. leading to the targeted phenylpropyl amines.

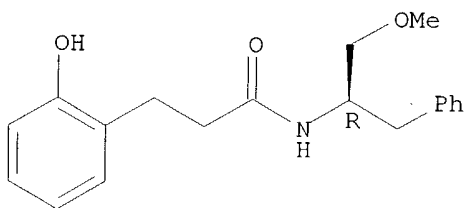
IT 221203-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of libraries of phenylpropyl amines and amides from dihydrocoumarin synthon)

RN 221203-10-7 HCA

CN Benzenepropanamide, 2-hydroxy-N-[(1R)-1-(methoxymethyl)-2-phenylethyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> D 158 11-47 CBIB ABS FHITSTR

L58 ANSWER 11 OF 47 HCA COPYRIGHT 2004 ACS on STN

130:144204 Modified amino acids as carriers for enhanced delivery of active agents. Leone-Bay, Andrea; Ho, Koc-kan; Sarubbi, Donald J.; Milstein, Sam J. (Emisphere Technologies, Inc., USA). U.S. US 5866536 A 19990202, 27 pp., Cont.-in-part of U.S. Ser. No. 414,654. (English). CODEN: USXXAM. APPLICATION: US 1997-798033 19970206. PRIORITY: US 1995-414654 19950331.

AB Carrier compds., compns., and dosage unit forms which are useful in the

delivery of active agents are provided. The present invention provides compds. such as 10-salicyloylaminodecanoic acid (I) for delivery of at least one active agent, including peptides, mucopolysaccharides, carbohydrates, or lipids. I prepared from 8-aminocaprylic acid and O-acetylsalicyloyl chloride was mixed with recombinant human growth hormone (rhGH) in a phosphate buffer solution. The composition was orally administered to rats at I 200 mg/kg and rhGH 3 mg/kg and delivery was evaluated by an ELISA assay for rhGH; mean peak serum levels of rhGH was .apprx.60.92 ng/mL as compared to <0.1 ng/mL for control group received a composition without I.

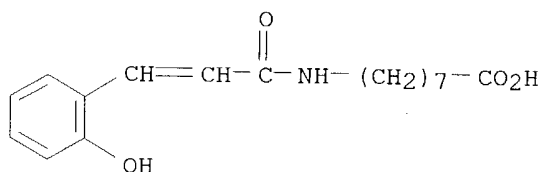
IT 183990-49-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of modified amino acids as carriers for enhanced delivery of active agents)

RN 183990-49-0 HCA

CN Octanoic acid, 8-[[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 12 OF 47 HCA COPYRIGHT 2004 ACS on STN

130:91738 A Chemical Approach To Illustrate the Principle of Signal Transduction Cascades Using the Avidin-Biotin System. Morpurgo, Margherita; Hofstetter, Heike; Bayer, Edward A.; Wilchek, Meir (Department of Biological Chemistry, The Weizmann Institute of Science, Rehovot, 76100, Israel). Journal of the American Chemical Society, 120(49), 12734-12739 (English) 1998. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB A new approach to illustrate the principle of signal transduction and to assemble protein multilayers is described. It is based on competing affinities of two different ligands for the same binding site of a protein. A low-affinity ligand can be attached covalently to the protein, where it will be buried in the binding site and thus be prevented to interact with other proteins that recognize it. However, if a high-affinity ligand (or a mol. containing this ligand) is added, it will displace the low-affinity ligand (which still remains covalently bound) from the binding site to the periphery. The low-affinity ligand is now available for interaction with other mols., thus providing the means through which to assemble multilayers of proteins by a recognition cascade. This principle was demonstrated using the protein avidin which binds two ligands, biotin and 4-hydroxyazobenzene-2-carboxylic acid (HABA), with markedly different affinities. Avidin was affinity labeled with HABA, the low-affinity ligand, to produce a red, covalently conjugated avidin-HABA derivative (red avidin). Anti-HABA antibodies failed to recognize HABA buried in the binding site of avidin. However, upon addition of the high-affinity ligand biotin, HABA was expelled from the binding site and immediately bound by the antibodies. Multilayer assemblies of HABAylated avidin and biotinylated anti-HABA antibodies could thus be constructed. BThis concept may find application in numerous fields, such as medicine, diagnostics, nanotechnol., and artificial

intelligence.

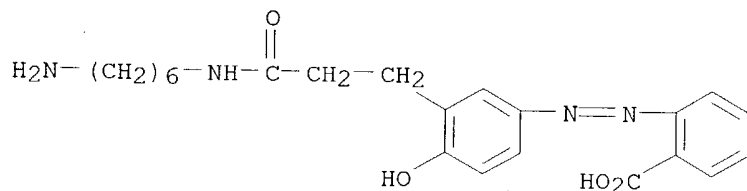
IT **219531-99-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 4-hydroxyazobenzene-2-carboxylic acid-labeled avidin for use in a model chemical signal transduction cascade using the avidin-biotin system)

RN 219531-99-4 HCA

CN Benzoic acid, 2-[[3-[3-[(6-aminohexyl)amino]-3-oxopropyl]-4-hydroxyphenyl]azo]- (9CI) (CA INDEX NAME)



L58 ANSWER 13 OF 47 HCA COPYRIGHT 2004 ACS on STN

127:322800 Modified amino acids for drug delivery. Leone-Bay, Andrea (Emisphere Technologies, Inc., USA; Leone-Bay, Andrea). PCT Int. Appl. WO 9736480 A1 19971009, 64 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US5128 19970318. PRIORITY: US 1996-17902 19960329.

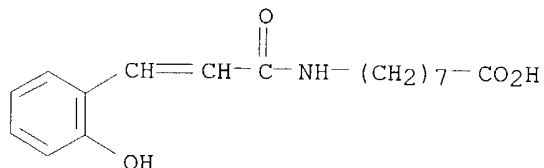
AB Modified amino acid compds. useful in the delivery of active agents are provided. E.g., 2HOC6H4CONH(CH2)7CO2H was prepared from 8-aminocaprylic acid and O-acetylsalicyloyl chloride. Also examples were give of a nol. of delivery agents enhancement of recombinant human growth hormone bioavailability administered s.c. in rats.

IT **183990-49-0P**

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses) (modified amino acids for drug delivery)

RN 183990-49-0 HCA

CN Octanoic acid, 8-[[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]amino]- (9CI) (CA INDEX NAME)



L58 ANSWER 14 OF 47 HCA COPYRIGHT 2004 ACS on STN

127:4988 A photo-sensitive protecting group for amines based on coumarin chemistry. Wang, Binghe; Zheng, Ailian (Dep. Chem., North Carolina State

Univ., Raleigh, NC, 27695, USA). Chemical & Pharmaceutical Bulletin, 45(4), 715-718 (English) 1997. CODEN: CPBTAL. ISSN: 0009-2363. Publisher: Pharmaceutical Society of Japan.

- AB There is a continuing need for the development of new protecting groups for amines which can be cleaved under conditions that are mild and fundamentally different from what are already available. In this paper, the authors report their studies in using o-hydroxy-trans-cinnamic acid as a photo-sensitive protecting group for amines. The design takes advantage of the trans-cis photo-isomerization and the ensuing facile lactonization of o-hydroxy-cis-cinnamic acid and derivs. The authors have found that both the protection and deprotection can be carried out in high yields for a variety of amines, HNRR' (R = H, Me, Et, R' = n-Pr, CH₂CH₂OH, CH₂Ph, cyclohexyl, etc.), with different structural features. The deprotection reaction uses low intensity UV light (365 nm), which is fundamentally different from the conditions used for the deprotection of other commonly used amino-protecting groups. Therefore, the method complements other available methods in allowing for selective manipulation of different functional groups in a complex organic mol.

IT 190366-77-9P

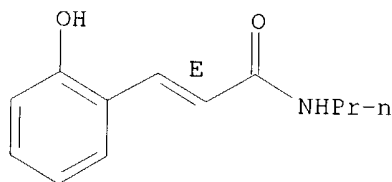
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(use of cinnamic acid as amine protecting group)

RN 190366-77-9 HCA

CN 2-Propenamide, 3-(2-hydroxyphenyl)-N-propyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L58 ANSWER 15 OF 47 HCA COPYRIGHT 2004 ACS on STN

126:321432 Coordinatively polymerized bilayer membranes prepared with an amphiphilic derivative of 2-thiazolylazophenol in water. Suh, Junghun; Shin, Seunghoon; Shim, Hyunbo (Department Chemistry, Seoul National University, Seoul, 151-742, S. Korea). Bulletin of the Korean Chemical Society, 18(2), 190-193 (English) 1997. CODEN: BKCSDE. ISSN: 0253-2964. Publisher: Korean Chemical Society.

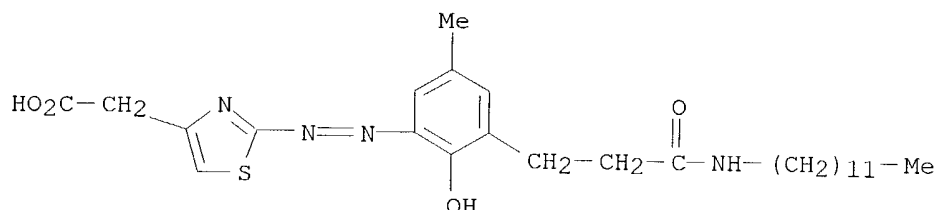
- AB In search of new amphiphiles that form coordinatively polymerized bilayer membranes (CPBMS) in H₂O, N-dodecyl-3-[2-hydroxy-3-(4-carboxymethyl-2-thiazolylazo)-5-methylphenyl]propanamide (I) was prepared. The bilayer membranes of I prepared in the presence of 2 equiv of NaOH were further sonicated in the presence of transition metal ions such as Ni(II), Cu(II), Co(II), or Co(III) at >80° to obtain CPBMs. The CPBMs of I were characterized by TEM, gel filtration, resistivity against disruption in aqueous EtOH, visible spectra, and release of entrapped 5(6)-carboxyfluorescein. Remarkable stabilization of the bilayer membranes through coordinative polymerization was evidenced by the resistivity of the Ni(II)-CPBM of I against disruption in 40% (volume/volume) EtOH upon incubation for 20 h.

IT 175613-63-5P, N-Dodecyl-3-[2-hydroxy-3-(4-carboxymethyl-2-thiazolylazo)-5-methylphenyl]propanamide

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(coordinatively polymerized bilayer membranes prepared with amphiphilic derivative of thiazolylazophenol in water)

RN 175613-63-5 HCA

CN 4-Thiazoleacetic acid, 2-[[3-[3-(dodecylamino)-3-oxopropyl]-2-hydroxy-5-methylphenyl]azo]- (9CI) (CA INDEX NAME)



L58 ANSWER 16 OF 47 HCA COPYRIGHT 2004 ACS on STN

124:262283 Coordinatively Polymerized Bilayer Membranes Prepared in Formamide. Suh, Junghun; Shim, Hyunbo (Department of Chemistry, Seoul National University, Seoul, 151-742, S. Korea). Langmuir, 12(9), 2323-4 (English) 1996. CODEN: LANGD5. ISSN: 0743-7463. Publisher: American Chemical Society.

AB A novel method was developed for preparation of bilayer membranes in polar organic

solvents, based on coordinative polymerization of N-dodecyl-3-[2-hydroxy-3-(4-(carboxymethyl)-2-thiazolylazo)-5-methylphenyl]propanamide (I) in the presence of Fe(II), Fe(III), or Co(II) ion in formamide. Formation of vesicular structure was supported by transmission electron micrographs, gel filtration, release of entrapped 5(6)-carboxyfluorescein, metal contents, and IR peaks for the azo linkage. Formation of bilayer membranes of I in formamide in the presence of the metal ions is attributed to the increased solvophilicity of the polar head upon complexation of the amphiphile to the metal ions and/or assemblage of the polar heads by coordinative polymerization

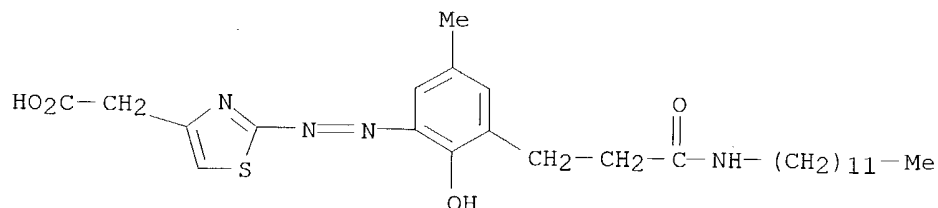
IT 175613-63-5DP, coordination polymers with cobalt or iron

RL: SPN (Synthetic preparation); PREP (Preparation)

(cobalt and iron coordination polymer bilayer membranes prepared in formamide)

RN 175613-63-5 HCA

CN 4-Thiazoleacetic acid, 2-[[3-[3-(dodecylamino)-3-oxopropyl]-2-hydroxy-5-methylphenyl]azo]- (9CI) (CA INDEX NAME)



L58 ANSWER 17 OF 47 HCA COPYRIGHT 2004 ACS on STN

123:34230 Coordinatively Polymerized Bilayer Membranes Prepared by Metal

Complexation of an Amphiphilic o,o'-Dihydroxyazobenzene Derivative. Suh, Junghun; Lee, Kyung Joon; Bae, Geuntaek; Kwon, Oh-Bin; Oh, Sezu (Department of Chemistry, Seoul National University, Seoul, 151-742, S. Korea). *Langmuir*, 11(7), 2626-32 (English) 1995. CODEN: LANGD5. ISSN: 0743-7463. Publisher: American Chemical Society.

AB As a novel method for stabilization of bilayer membranes, coordinative polymerization of bilayer membranes of an amphiphile containing 2 ligating sites has

been developed. Complexation of Fe(II), Fe(III), Co(II), or Co(III) ion with the bilayer membranes of an amphiphile which contains an o,o'-dihydroxyazobenzene moiety as the rigid segment leads to the formation of coordinatively polymerized bilayer membranes. The coordinatively polymerized bilayer membranes are characterized by transmission electron microscopy, gel filtration, phase transition, release of entrapped 5(6)-carboxyfluorescein, visible spectra, IR spectra, and elec. conductivity. Helical superstructures are obtained with Co(II) ion, although the amphiphilic does not contain any chiral center, whereas rodlike structures are formed with Fe(II), Fe(III), or Co(III) ion. Stabilization of bilayer membranes upon coordinative polymerization is demonstrated by enhanced resistivity to disruption in aqueous ethanol. In addition, the fluidity and rigidity of the coordinatively polymerized bilayer membranes can be balanced by changing the metal content.

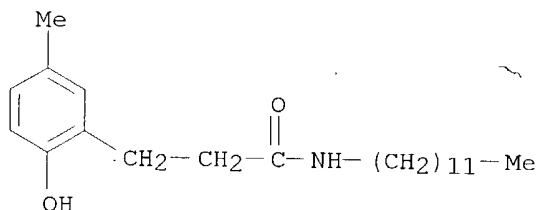
IT **163983-31-1P**, 3-(2-Dodecylcarbamoyl-ethyl)-2-hydroxy-5-methylbenzene

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; coordinatively polymerized bilayer membranes prepared by metal complexation of amphiphilic dihydroxyazobenzene derivative)

RN 163983-31-1 HCA

CN Benzenepropanamide, N-dodecyl-2-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



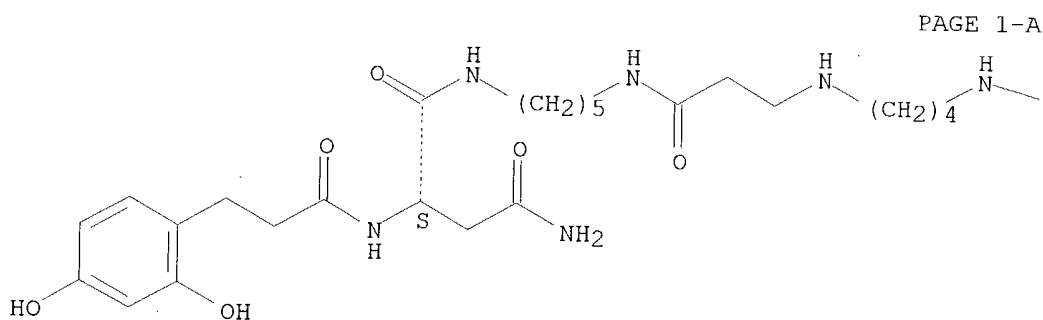
L58 ANSWER 18 OF 47 HCA COPYRIGHT 2004 ACS on STN

122:284360 Structural characterization of glutaminergic blocker spider toxins by high-energy collision charge-remote fragmentations. Fujita, Tsuyoshi; Itagaki, Yasuhiro; Naoki, Hideo; Nakajima, Terumi; Hagiwara, Ken'ichi (Suntory Inst. Bioorg. Res., Osaka, 618, Japan). *Rapid Communications in Mass Spectrometry*, 9(5), 365-71 (English) 1995. CODEN: RCMSEF. ISSN: 0951-4198. Publisher: Wiley.

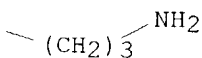
AB Spider venom gland stores various glutaminergic blockers such as acylpolyamines, besides proteins and peptides. A method is described for structure determination of these acylpolyamines using fast-atom bombardment and four-sector tandem mass spectrometry. The collision-induced dissociation (CID) spectra of protonated mol. ions of synthetic model compds. show only a small number of weak, sequence-related product ions. But, unlike the CID spectra of [M + H]⁺ ions, dissociation of sodium-attached mol. ions leads to charge-remote fragmentations and provides intense sequence-related product

ions.
 IT **126992-57-2**
 RL: PRP (Properties)
 (structural characterization of glutaminergic blocker spider toxins by high-energy collision charge-remote fragmentations)
 RN 126992-57-2 HCA
 CN Butanediamide, N1-[5-[[3-[[4-[(3-aminopropyl)amino]butyl]amino]-1-oxopropyl]amino]pentyl]-2-[[3-(2,4-dihydroxyphenyl)-1-oxopropyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

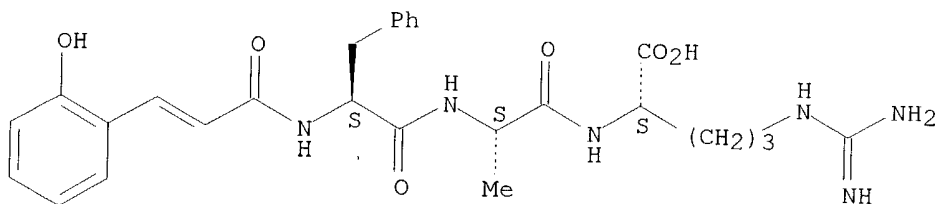


PAGE 1-B



L58 ANSWER 19 OF 47 HCA COPYRIGHT 2004 ACS on STN
 122:154747 Novel fluorogenic substrate of carboxypeptidase H --
 o-coumaroyl-phenylalanyl-alanyl-arginine. Pozdnev, V. F.; Varlamov, O. L.; Grigoriants, O. O.; Gomaskov, O. A. (Inst. Biomed. Chem., Moscow, Russia). Bioorganicheskaya Khimiya, 20(4), 406-12 (Russian) 1994. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.
 AB A new fluorogenic substrate of carboxypeptidase H, Cum-Phe-Ala-Arg-Oh, is hydrolyzed by this enzyme to give Cum-Phe-Ala-OH, which is completely extracted by chloroform from the reaction mixture and whose fluorescence increases remarkably by the presence of triethylamine. When the hydrolysis of the novel substrate is compared with Dns-Phe-Ala-Arg-OH, the former has Km twice as low (30 μM) and Kcat four times as high (5.8 s⁻¹). Activation of the enzyme by Co²⁺ in reactions with the two substrates was also studied. The novel substrate is useful for the enzyme's assay in homogenates of various animal tissues.
 IT **161258-31-7P**
 RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (fluorogenic peptide substrate for carboxypeptidase determination)
 RN 161258-31-7 HCA
 CN L-Arginine, N2-[N-[N-[3-(2-hydroxyphenyl)-1-oxo-2-propenyl]-L-phenylalanyl]-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L58 ANSWER 20 OF 47 HCA COPYRIGHT 2004 ACS on STN

116:27408 Microbial extracellular enzyme activity: a new key parameter in aquatic ecology. Hoppe, Hans Georg (Abt. Mar. Mikrobiol., Inst. Meereskd., Kiel, D-2300, Germany). Microb. Enzymes Aquat. Environ., [Pap. Workshop Enzymes Aquat. Environ.], 1st, Meeting Date 1989, 60-83. Editor(s): Chrost, Ryszard J. Springer: New York, N. Y. (English) 1991. CODEN: 57KHAF.

AB This study provides preliminary data concerning bacterial enzymic activity on organic and inorg. surfaces to support the theory that free bacteria may benefit from the hydrolysis activity of attached bacteria. Studies concerning the relationship between extracellular enzyme activities of attached and free-living bacteria were conducted using natural detritus materials and submerged glass slides near the coast of the Kiel Fjord (Germany).

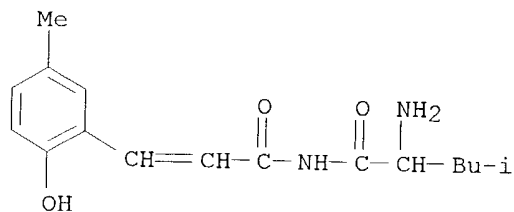
IT 138087-26-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(enzymic hydrolysis of, by attached and free-living bacteria, organic matter degradation in relation to, in Kiel Fjord, Germany)

RN 138087-26-0 HCA

CN Pentanamide, 2-amino-N-[3-(2-hydroxy-5-methylphenyl)-1-oxo-2-propenyl]-4-methyl- (9CI) (CA INDEX NAME)



L58 ANSWER 21 OF 47 HCA COPYRIGHT 2004 ACS on STN

116:10732 Significance of extracellular enzymes for organic matter degradation and nutrient regeneration in small streams. Marxsen, Juergen; Witzel, Karl Paul (Max-Planck Inst. Limnol., Schlitz, D-6407, Germany). Microb. Enzymes Aquat. Environ., [Pap. Workshop Enzymes Aquat. Environ.], 1st, Meeting Date 1989, 270-85. Editor(s): Chrost, Ryszard J. Springer: New York, N. Y. (English) 1991. CODEN: 57KHAF.

AB Methodol. investigations into the suitability of methylumbelliferyl compds. for studying enzyme activities in different streams and stream habitats were made. Results obtained with this technique for degradation of

organic matter and nutrient regeneration in 3 streams (Breitenbach, Rohrwiesenbach, Jossa) near Frankfurt/Main, Germany, are presented.

IT **138628-71-4**

RL: PROC (Process)

(substrate, for determining extracellular enzyme activity on stream water and

sediments, organic matter microbial degradation in relation to, of Breitenbach

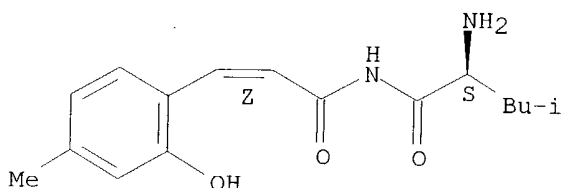
and RohrivIEWSinbach and Jossa rivers, Germany)

RN 138628-71-4 HCA

CN Pentanamide, 2-amino-N-[3-(2-hydroxy-4-methylphenyl)-1-oxo-2-propenyl]-4-methyl-, [S-(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

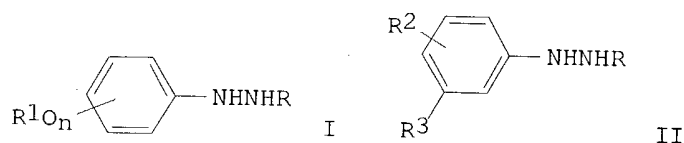
Double bond geometry as shown.



L58 ANSWER 22 OF 47 HCA COPYRIGHT 2004 ACS on STN

115:38568 Silver halide photographic material containing hydrazine enhancing the contrast without generating developer fog. Usagawa, Yasushi; Ishii, Fumio (Konica Co., Japan). Jpn. Kokai Tokkyo Koho JP 02285342 A2 19901122 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1989-106899 19890426.

GI



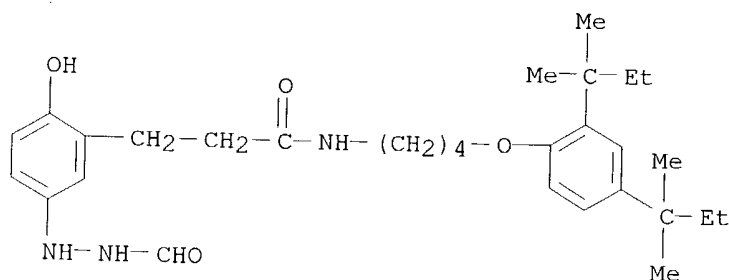
AB A photog. material having ≥ 1 Ag halide emulsion layer on a support contains a compound I (R = formyl, acyl, sulfonyl, carbamoyl, sulfamoyl, alkoxy carbamoyl, thioacyl; R1 = alkyl with non-diffusible group; R1On group substitutes at o- or p-site of the Ph group; n = 0, 1) or II (R2 = OH, alkyl, amino, substitutes at o- or p-site of the Ph group; R3 = alkyl, ≥ 1 R1 and R2 contains non-diffusible group or a group promoting adsorption to Ag halide). The compds. enhance contrast without inducing developer fog or black peppers. Thus, Ag(Br,Cl) emulsion (Br/Cl = 40/60, monodispersed, Rh and Ir salt-incorporated) was added by a hydrazine I [R = MeOCH2CO, R1 = N-(cyclohexylamido)-N-(cyclohexyl)-aminocarbonylmethyl, n = 1], and applied on a film base to make a high contrast photog. film useful for photomech. process.

IT **134719-47-4**

RL: TEM (Technical or engineered material use); USES (Uses)
(photog. emulsion containing, for high contrast image)

RN 134719-47-4 HCA

CN Benzenepropanamide, N-[4-[2,4-bis(1,1-dimethylpropyl)phenoxy]butyl]-5-(2-formylhydrazino)-2-hydroxy- (9CI) (CA INDEX NAME)



L58 ANSWER 23 OF 47 HCA COPYRIGHT 2004 ACS on STN

114:246882 Derivatives of arylalkylamines. XXVI. Arylation of a cinnamate ester by fluorobenzene and o-bromophenol. Balayan, R. S.; Asoyan, E. L.; Pogosyan, A. V.; Markaryan, E. A. (Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR). Armyanskii Khimicheskii Zhurnal, 43(10), 672-8 (Russian) 1990. CODEN: AYKZAN. ISSN: 0515-9628. OTHER SOURCES: CASREACT 114:246882.

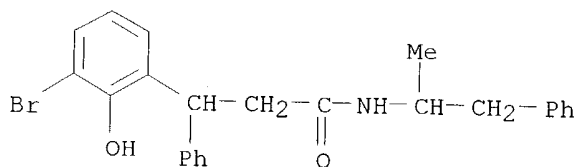
AB Arylation of PhCH:CHR (R = CO₂Me, cyano) PhF and o-BrC₆H₄OH in PhNO₂ containing AlCl₃ gave 32-45.4% R₁CHPhCH₂R [I; R₁ = 4-FC₆H₄, 3,2-Br(HO)C₆H₃], 11% 3-(p-fluorophenyl)-1-indanone, and 8-bromo-4-phenyl-3,4-dihydrocoumarin. Saponifying I (R = CO₂Me) gave 77-93% I' (R = CO₂H), which were amidated with SOCl₂ and R₂NH₂ [R₂ = PhCH₂CHMe, (MeO)₂C₆H₃CH₂CH₂, Ph₂CHCH₂CH₂, Ph₂CHCH₂CHMe] in refluxing C₆H₆ containing pyridine to give 8 R₁CHPhCH₂CONHR₂ (II) in 63-96% yield. Reducing II (R₁ = 4-FC₆H₄) with LiAlH₄ in dry EtO gave 55-80% 4-FC₆H₄CHPhCH₂CH₂NHR₂.

IT 134101-82-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 134101-82-9 HCA

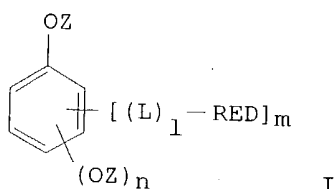
CN Benzenepropanamide, 3-bromo-2-hydroxy-N-(1-methyl-2-phenylethyl)-β-phenyl- (9CI) (CA INDEX NAME)



L58 ANSWER 24 OF 47 HCA COPYRIGHT 2004 ACS on STN

114:33030 Polymeric color mixing inhibitor-containing photographic material. Nakamura, Yoshisada; Ono, Shigetoshi (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 02115838 A2 19900427 Heisei, 28 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-268078 19881026.

GI



AB The title photog. material contains a polymer obtained by the co-condensation of ≥ 1 I [L = divalent linking group; RED = group undergoing a redox reaction with oxidized developing agent; Z = H, group removal via reaction with alkali; l = 1, 2; m = 1, 2; n = 1-4; m + n ≤ 5] with ≥ 1 R₂CO [R = H, CO₂H, formyl, alkyl, aryl, heterocyclyl, acyl, sulfonamide] in the presence of an acid or basic catalyst. The above polymer serves to inhibit color mixing, and has good shelf-life.

IT **131075-45-1**

RL: USES (Uses)

(photog. color mixing inhibitor, color paper using)

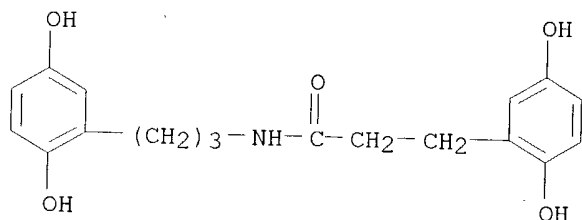
RN 131075-45-1 HCA

CN Benzenepropanamide, N-[3-(2,5-dihydroxyphenyl)propyl]-2,5-dihydroxy-, polymer with N-(2,5-dihydroxyphenyl)-N'-[2-hydroxy-5-[(methylsulfonyl)amino]phenyl]-1,3-benzenedisulfonamide and octanal (9CI) (CA INDEX NAME)

CM 1

CRN 131075-44-0

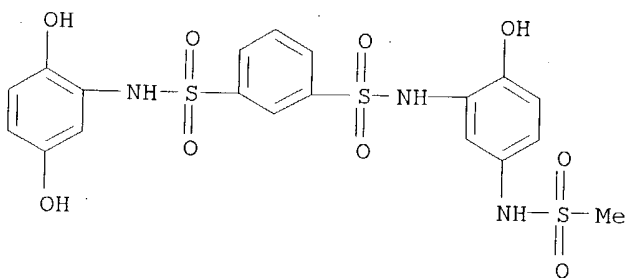
CMF C18 H21 N O5



CM 2

CRN 131046-50-9

CMF C19 H19 N3 O9 S3



CM 3

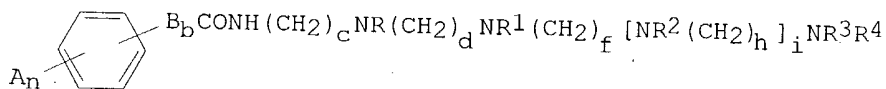
CRN 124-13-0

CMF C8 H16 O

OHC-(CH₂)₆-Me

L58 ANSWER 25 OF 47 HCA COPYRIGHT 2004 ACS on STN
 113:226431 Preparation of biocidal polyamine amides. Usherwood, Peter Norman
 Russell; Bycroft, Barrie Walsham; Blagbrough, Ian Stuart; Mather, Alan
 John (National Research Development Corp., UK). Brit. UK Pat. Appl. GB
 2222402 A1 19900307, 32 pp. (English). CODEN: BAXXDU. APPLICATION: GB
 1989-19564 19890830. PRIORITY: GB 1988-20472 19880830.

GI



I

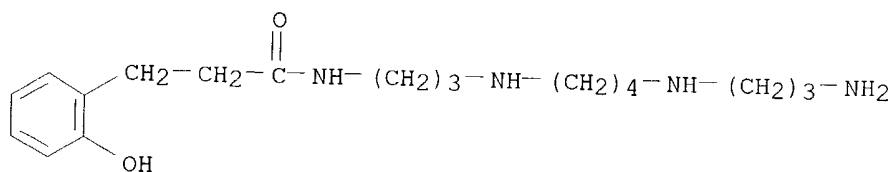
AB The polyamine amides I [A = OH, alkoxy, etc.; B = (un)substituted C1-6
 aliphatic hydrocarbon group; R-R4 = H, alkyl, cycloalkyl; NR3R4 =
 heterocyclyl; a = 0, 1-5; b = 0, 1; c, d, f, h = 2-6; i = 0, 1] are prepared
 as agricultural pesticides. A mixture of 2-hydroxyphenylacetic acid,
 1,2-dimethoxyethane, dicyclohexyl carbodiimide, and DME was kept at
 25° for 3 h, followed by filtration. The filtrate was treated with
 spermine in DME/DMF to give N-(2-hydroxyphenylacetyl)spermine (II). II
 antagonized the complex formed by the invertebrate L-quisqualate sub-type
 L-glutamate receptor and its ion channel, in the elec.-stimulated
 retractor unguis muscle of the locust (*Schistocerca gregaria*). The mean
 inhibitory concentration was 6.2+10⁻⁵ M II.

IT 130210-33-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except
 adverse); BSU (Biological study, unclassified); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as pesticide)

RN 130210-33-2 HCA

CN Benzenepropanamide, N-[3-[[4-[(3-aminopropyl)amino]butyl]amino]propyl]-2-
 hydroxy- (9CI) (CA INDEX NAME)



L58 ANSWER 26 OF 47 HCA COPYRIGHT 2004 ACS on STN

107:77005 Method for converting ether groups to hydroxyl groups and ester groups to acid groups. King, Patrick F. (Polaroid Corp., USA). U.S. US 4652635 A 19870324, 8 pp. Cont.-in-part of U.S. Ser. No. 490,773, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1984-621060 19840615. PRIORITY: US 1983-490773 19830502.

AB A process for dealkylation of alkyl or aryl ethers and hydrolysis of alkyl or aryl esters by treating them successively with a 2-halo-1,3,2-benzodioxaborole and H₂O is described. A mixture of Me 1-naphthaleneacetate and 2-bromo-1,3,2-benzodioxaborole in CH₂Cl₂ was stirred for 24 h at room temperature and subsequently treated with H₂O to give 60% 1-naphthaleneacetic acid. The method was used to deblock a variety of protected dye developers.

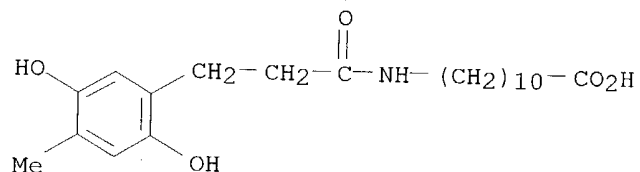
IT 109547-22-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by dealkylation and hydrolysis of ether-ester derivative with bromobenzodioxaborole and water)

RN 109547-22-0 HCA

CN Undecanoic acid, 11-[[3-(2,5-dihydroxy-4-methylphenyl)-1-oxopropyl]amino]-(9CI) (CA INDEX NAME)



L58 ANSWER 27 OF 47 HCA COPYRIGHT 2004 ACS on STN

103:203595 Application of anisotropic photocleavage of head-to-head type cyclobutane compounds. Yonezawa, Noriyuki; Yamashita, Takashi; Kanoe, Toshio; Saigo, Kazuhiko; Hasegawa, Masaki (Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan). Industrial & Engineering Chemistry Product Research and Development, 24(4), 593-8 (English) 1985. CODEN: IEPRA6. ISSN: 0196-4321.

AB The cyclobutane ring in head-to-head coumarin dimers and their lactone-opened derivs. photocleaves in 3 different modes: sym., asym., and competitive. On the basis of the structural factors governing these pathways, controlling the mode of the photocleavage reaction of some head-to-head cyclobutane compds. was put into practice. The polyamide derived from coumarin dimer was transformed to another linear polyamide by exclusively asym. photocleavage of the cyclobutane rings in the main chain. The pH of a solution containing monoanilide derivs. of coumarin dimer was

changed by photoirradn. due to the cleavage of the cyclobutane ring followed by spontaneous relactonization. An unsym. substituted stilbene

was synthesized from a substituted cinnamic anhydride by intramol. photocycloaddn. and asym. photocleavage.

IT **98977-46-9P**

RL: PREP (Preparation)

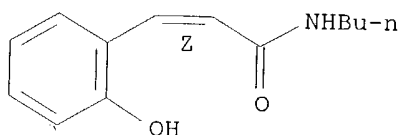
(formation and reaction of, in relactonization of coumaric acid derivative, photochem. pH modification of solution containing lactone-opened derivative of

coumarin dimer in relation to)

RN 98977-46-9 HCA

CN 2-Propenamamide, N-butyl-3-(2-hydroxyphenyl)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L58 ANSWER 28 OF 47 HCA COPYRIGHT 2004 ACS on STN

103:123210 Lithiation in flavones, chromones, coumarins, and benzofuran derivatives. Costa, Ana M. B. S. R. C. S.; Dean, Francis M.; Jones, Michael A.; Varma, Rajender S. (Robert Robinson Lab., Univ. Liverpool, Liverpool, L69 3BX, UK). Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (4), 799-808 (English) 1985. CODEN: JCPRB4. ISSN: 0300-922X. OTHER SOURCES: CASREACT 103:123210.

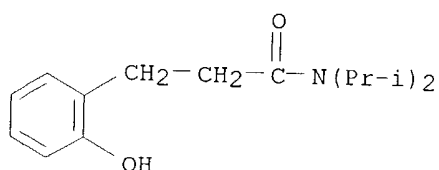
AB Flavones were lithiated in the 3-position by $\text{LiN}(\text{CHMe}_2)_2$ in THF at -78° to give stable derivs. which were readily converted to the corresponding carboxy, ethoxycarbonyl, mercapto, methylthio, trimethylsilyl, hydroxy, or other derivs. E.g., treatment of flavone with $\text{LiN}(\text{CHMe}_2)_2$ in THF at -78° gave 3-lithioflavone which reacted with CO_2 to give 92% 3-flavonecarboxylic acid. Benzofurans were preferentially lithiated at the 2-position; where this was blocked lithiation occurred in the 3-position in the presence of an activating group. Ring-opening of benzofurans occurred in some cases giving acetylenic phenols directly. Chromenes were lithiated at positions 2 and 3, depending on substitution. Coumarins generally behaved as esters and gave the corresponding amides with $\text{LiN}(\text{CHMe}_2)_2$, except for 4-methoxycoumarin which underwent lithiation in the 3-position. Deprotonation in the 32-position in ethers occurs easily only when there is an ether link antiperiplanar to the proton removed. The lithiated species are really unstable intermediates in trans eliminations leading to alkyne derivs.

IT **77037-51-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77037-51-5 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L58 ANSWER 29 OF 47 HCA COPYRIGHT 2004 ACS on STN

103:67458 Kinetics and mechanisms of hydroxyl radical-induced crosslinks between phenylalanine peptides. Simic, Michael G.; Gajewski, Ewa; Dizdaroglu, Miral (Cent. Radiat. Res., Natl. Bur. Stand., Gaithersburg, MD, 20899, USA). Radiation Physics and Chemistry, 24(5-6), 465-73 (English) 1984. CODEN: RPCHDM. ISSN: 0146-5724.

AB Reactions of $\bullet\text{OH}$ radicals with phenylalanine (Phe) and its homopeptides, i.e., L-Phe-L-Phe and L-Phe-L-Phe-L-Phe, in N_2O -saturated aqueous solns. were investigated by pulse radiolysis, high-performance liquid chromatog., capillary gas chromatog., and mass spectrometry. For identification of radiation-induced products, samples of irradiated Phe and HCl -hydrolyzates of its irradiated homopeptides were trimethylsilylated and analyzed by capillary gas chromatog.-mass spectrometry. Mass spectra of the trimethylsilylated products revealed the formation of o-, m-, and p-tyrosines and biphenyl-type dimers. The G values of these products were also determined by gas chromatog. Mechanisms of product formation were discussed.

IT 97539-96-3

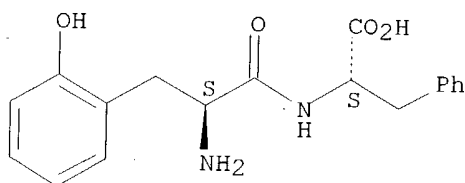
RL: FORM (Formation, nonpreparative)

(formation of, from phenylalanine peptides after radiolysis)

RN 97539-96-3 HCA

CN L-Phenylalanine, N-(2-hydroxy-L-phenylalanyl)- (9CI) (CA INDEX NAME)

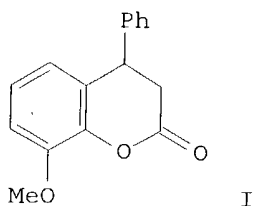
Absolute stereochemistry.



L58 ANSWER 30 OF 47 HCA COPYRIGHT 2004 ACS on STN

100:102836 Arylalkylamine derivatives. XIX. Synthesis of some 3-(2-hydroxy-3-methoxyphenyl)-3-phenyl-N-(arylalkyl)propylamines and their biological activity. Balayan, R. S.; Akopyan, M. G.; Kaltrikyan, A. A.; Markaryan, E. A. (Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR). Armyanskii Khimicheskii Zhurnal, 36(10), 653-7 (Russian) 1983. CODEN: AYKZAN. ISSN: 0515-9628. OTHER SOURCES: CASREACT 100:102836.

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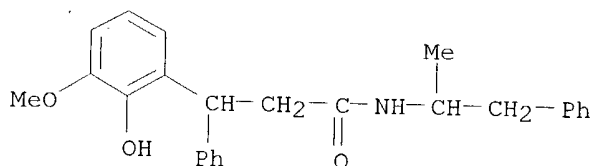
AB PhCH:CHCO₂Me reacted with guaiacol in PhNO₂ containing AlCl₃ at 80° to give 51.4% dihydrocoumarin I via cyclization of the intermediate 2,3-HO(MeO)C₆H₃CHPhCH₂COX (II; X = OMe). Saponifying I gave 85.4% II (X = OH), which reacted with SOCl₂ to give II (X = Cl) and then with RNH₂ [R = PhCH₂CHMe, 3,4-(MeO)₂C₆H₃, Ph₂CHCH₂CH₂, Ph₂CHCH₂CHMe, PhCH₂CH₂CHMe] to give the corresponding II (X = NHR) in 72-92% yield. Reducing the latter with LiAlH₄ gave 50-65% 2,3-HO(MeO)C₆H₃CHPhCH₂CH₂NHR (same R), which have pronounced and long-term α-sympatholytic activity (no data).

IT **89027-99-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of, amine by)

RN 89027-99-6 HCA

CN Benzenepropanamide, 2-hydroxy-3-methoxy-N-(1-methyl-2-phenylethyl)-β-phenyl- (9CI) (CA INDEX NAME)



L58 ANSWER 31 OF 47 HCA COPYRIGHT 2004 ACS on STN

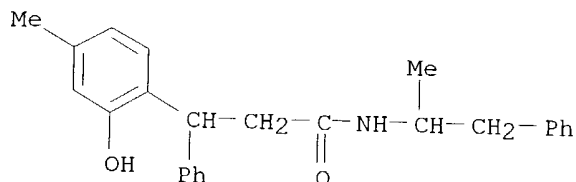
100:34210 Arylalkylamine derivatives. XVIII. Synthesis and pharmacological activity of some 3-[2-hydroxy-4(or 5)-methylphenyl]-3-phenyl-N-(arylalkyl)propylamines. Balayan, R. S.; Akopyan, M. G.; Kaltrikyan, A. A.; Avakyan, O. M.; Markaryan, E. A. (Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR). Armyanskii Khimicheskii Zhurnal, 36(7), 451-6 (Russian) 1983. CODEN: AYKZAN. ISSN: 0515-9628. OTHER SOURCES: CASREACT 100:34210.

AB Arylation of PhCH:CHCO₂Me with p- and m-cresol in the presence of AlCl₃ gave 59.4% 6- and 53.4% 7-methyl-4-phenyl-3,4-dihydrocoumarin, resp., which were saponified with NaOH to give 83.7% 5,2- and 77.5% 4,2-Me(HO)C₆H₃CHPhCH₂CO₂H. Treating these with SOCl₂ and then RNH₂ [R = PhCH₂CHMe, 3,4-(MeO)₂C₆H₃CH₂CH₂, PhCH₂CH₂CHMe, Ph₂CHCH₂CH₂, Ph₂CHCH₂CHMe] in refluxing absolute C₆H₆ gave the corresponding Me(HO)C₆H₃CHPhCH₂CONHR (I), which were also formed in 60-91% yield directly from the dihydrocoumarins and RNH₂ in refluxing C₆H₆. LiAlH₄ reduction of I in absolute Et₂O gave, after acidification, 49-86% 5,2- and 4,2-Me(HO)C₆H₃CHPhCH₂CH₂NHR·HCl, which showed significant α-adrenoblocking activity.

IT **88407-31-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, with lithium aluminum hydride)

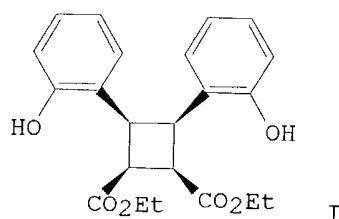
RN 88407-31-2 HCA

CN Benzenepropanamide, 2-hydroxy-4-methyl-N-(1-methyl-2-phenylethyl)- β -phenyl- (9CI) (CA INDEX NAME)

L58 ANSWER 32 OF 47 HCA COPYRIGHT 2004 ACS on STN

99:121855 Symmetric and asymmetric photocleavage of the cyclobutane rings in head-to-head coumarin dimers and their lactone-opened derivatives. Yonezawa, Noriyuki; Yoshida, Tsuyoshi; Hasegawa, Masaki (Dep. Synth. Chem., Univ. Tokyo, Tokyo, 113, Japan). Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (5), 1083-6 (English) 1983. CODEN: JCPRB4. ISSN: 0300-922X.

GI



AB Photochem. cleavage of head-to-head coumarin dimers and their lactone-opened derivs. on irradiation with 277 nm light gave 2 mols. of coumarin derivative by sym. fission and/or (2-HOC6H4CH:)2 (I) and fumaric/maleic acid derivs. by asym. fission. E.g., irradiation of cyclobutane II in EtOH for 1 h gave a 36:64 mixture of the sym. cleavage product 2-HOC6H4CH:CHCO2Et and asym. cleavage products I and (EtO2CCH:)2, quant. The direction of cleavage is mainly determined by the basic structure of the substrate, the photocleavage proceeding exclusively with retention of the ring structure when there is a stable 5- or 6-membered ring fused to the cyclobutane. Steric repulsions between substituents on the cyclobutane ring exert a secondary effect.

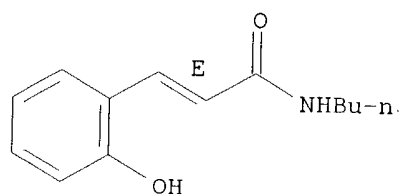
IT 86774-83-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by photolysis of lactone-opened coumarin dimer)

RN 86774-83-6 HCA

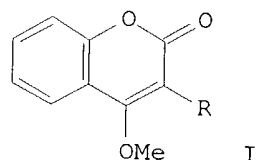
CN 2-Propenamide, N-butyl-3-(2-hydroxyphenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L58 ANSWER 33 OF 47 HCA COPYRIGHT 2004 ACS on STN
94:139563 β -Deprotonation by lithium diisopropylamide. Vinyl carbanions from oxygen heterocycles in the synthesis of carboxylic acids in the benzofuran, flavone, and coumarin series and in the regiospecific acylation of 2,6-dimethylchromone. Costa, Ana M. B. S. R. C. S.; Dean, Francis M.; Jones, Michael A.; Smith, Dennis A.; Varma, Rajender S. (Robert Robinson Lab., Univ. Liverpool, Liverpool, L69 3BX, UK). Journal of the Chemical Society, Chemical Communications (24), 1224-6 (English) 1980. CODEN: JCCCAT. ISSN: 0022-4936. OTHER SOURCES: CASREACT 94:139563.

GI



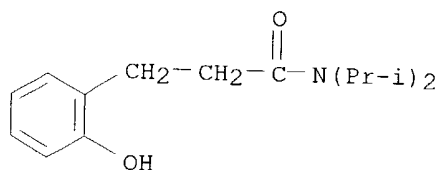
AB $\text{LiN}(\text{CHMe}_2)_2$, at -70° deprotonated benzofuran, at the α -position in the absence of activating groups, whereas, in the presence of activating groups, the β -proton was removed. In flavone and 4-methoxycoumarin (I), β -deprotonation occurred readily and the carbanions formed were easily carboxylated giving previously inaccessible acids. E.g., I ($\text{R} = \text{H}$) underwent deprotonation and carboxylation to give the acid I ($\text{R} = \text{CO}_2\text{H}$). In 2,6-dimethylchromone, β -deprotonation was kinetically favored allowing 3-acylation to be achieved.

IT 77037-51-5p

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77037-51-5 HCA

CN Benzenepropanamide, 2-hydroxy-N,N-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L58 ANSWER 34 OF 47 HCA COPYRIGHT 2004 ACS on STN

93:46148 Derivatives of arylalkylamines. XIV. The 3-(o- or p-hydroxyphenyl)-3-phenyl-N-(phenylisopropyl)propylamines. Balayan, R. S.; Markaryan, E. A. (Inst. Tonk. Org. Khim. im. Mndzhoyana, Yerevan, USSR). Armyanskii Khimicheskii Zhurnal, 32(8), 673-77 (Russian) 1979. CODEN: AYKZAN. ISSN: 0515-9628.

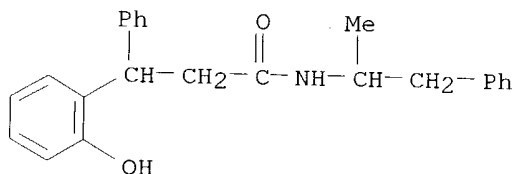
AB PhCH:CHCO₂Me condensed with PhOH in PhNO₂ containing AlCl₃ at 70° to give 52.4% o-HOC₆H₄CHPhCH₂CO₂Me and 19.3% 4-phenyl-3,4-dihydrocoumarin, both of which were saponified to o-HOC₆H₄CHPhCH₂CO₂H (I) in ≤76.3% yield. I and its paraisomer were amidated with PhCH₂CHMeNH₂ in 85.70-90.3% yield via the acid chlorides, and the amides were reduced with LiAlH₄ to give 18.3% o- and 50.4% p-HOC₆H₄CHPhCH₂CH₂NHCHMeCH₂Ph, resp.

IT 67792-01-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, with lithium aluminum hydride)

RN 67792-01-2 HCA

CN Benzenepropanamide, 2-hydroxy-N-(1-methyl-2-phenylethyl)-β-phenyl- (9CI) (CA INDEX NAME)



L58 ANSWER 35 OF 47 HCA COPYRIGHT 2004 ACS on STN

91:74324 3-Ortho(para)-hydroxyphenyl-3-phenyl-N-(phenylisopropyl)propylamines and salts thereof. Markarian, E. A.; Balaian, R. S.; Avakian, O. M.; Kaltrikian, A. A. (Mndzhoyan, A. L., Institute of Fine Organic Chemistry, Armenian Academy of Sciences, S.S.R., USSR). Brit. GB 1541197 19790221, 12 pp. (English). CODEN: BRXXAA. APPLICATION: GB 1977-5679 19770211.

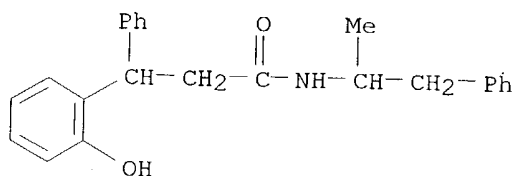
AB The preparation is described of RC₆H₄CHPh(CH₂)₂NHCHMeCH₂Ph. (HX)_n [I; R = 2-, 4-HO; X = Cl, Br, O₂CCH:CHCO₂H, O₂CCH(OH)CH(OH)CO₂H; n = 0, 1], which have selective coronary dilative activity. Thus, I (R = 2-HO, X = Cl, n = 1) was prepared from 2-HOC₆H₄CHPhCH₂CO₂H by sequential treatment with SOCl₂, PhCH₂CHMeNH₂/pyridine, LiAlH₄, and HCl. The pharmacol. activities of I were determined in rats, cats, and isolated organs. I (R = 4-HO, X = Cl, n = 1) (II) showed adrenolytic and sympatholytic activity and caused lasting depletion of cardiac endogenic catecholamines. LD₅₀ for II is 260 mg/kg i.p. in mice.

IT 67792-01-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

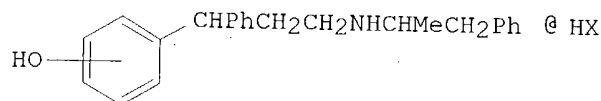
RN 67792-01-2 HCA

CN Benzenepropanamide, 2-hydroxy-N-(1-methyl-2-phenylethyl)-β-phenyl- (9CI) (CA INDEX NAME)



L58 ANSWER 36 OF 47 HCA COPYRIGHT 2004 ACS on STN
 89:146607 3-o(p)-Hydroxyphenyl-3-phenyl-N-(phenylisopropyl)propylamines and their salts. Markaryan, E. A.; Balayan, R. S.; Avakyan, O. M.; Kaltrikyan, A. A. (Institute of Fine Organic Chemistry, Academy of Sciences, Armenian S.S.R., USSR). Ger. Offen. DE 2701851 19780720, 28 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1977-2701851 19770118.

GI



I

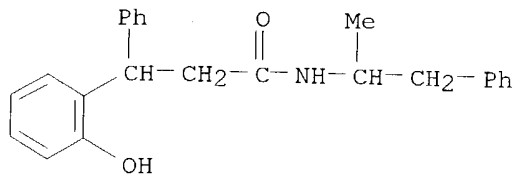
AB The title compds. I (X = Cl, Br, cis-HO₂CCH:CHCO₂, HO₂CCH(OH)CH(OH)CO₂; o- or p-OH), useful as coronary vasodilators, sympatholytics, and adrenolytics (extensive data tabulated), were prepared from o-(p)-HOC₆H₄CHPhCH₂CO₂H in 4 steps. Thus, o-HOC₆H₄CHPhCH₂CO₂H was converted to its acid chloride with SOCl₂, the product amidated with H₂NCHMeCH₂Ph in pyridine and C₆H₆, and the resultant o-HOC₆H₄CHPhCH₂CONHCHMeCH₂Ph reduced with LiAlH₄ in Et₂O to give 58% o-HOC₆H₄CHPhCH₂CH₂NHCHMeCH₂Ph, which was converted to its HCl, HBr, tartrate, and maleate salts.

IT **67792-01-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)

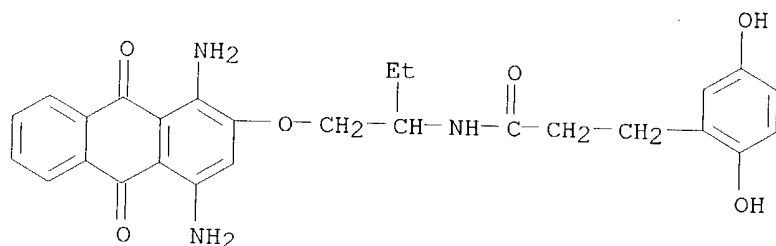
RN 67792-01-2 HCA

CN Benzenepropanamide, 2-hydroxy-N-(1-methyl-2-phenylethyl)-β-phenyl-
 (9CI) (CA INDEX NAME)

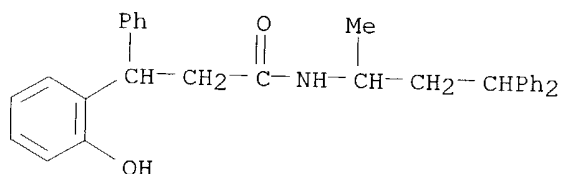


L58 ANSWER 37 OF 47 HCA COPYRIGHT 2004 ACS on STN
 88:50013 Base-induced rearrangements of mesityl thienyl sulfones. Truce, William E.; VanGemert, Barry; Brand, William W. (Dep. Chem., Purdue Univ., West Lafayette, IN, USA). Journal of Organic Chemistry, 43(1), 101-5 (English) 1978. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 88:50013.

- AB 5-Mesitylsulfonyl-2-methyl- and 2-mesitylsulfonylthiophene (I) undergo the Truce-Smiles rearrangement. The thienyl unit migrates with a change in orientation regardless of the base/solvent system used. The chemical of I is complicated by the acidity of the open α -position, with 2 equiv base being required for rearrangement. Monometalated I on the other hand, slowly decomposes to give 1,3,5-Me₃C₆H₂SO₂H as the only isolable product. A modified Michael addition- β -elimination mechanism is proposed.
- IT **6398-89-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and decomposition of)
- RN 6398-89-6 HCA
- CN Benzenepropanamide, N-[1-[[[(1,4-diamino-9,10-dihydro-9,10-dioxo-2-anthracenyl)oxy]methyl]propyl]-2,5-dihydroxy- (9CI) (CA INDEX NAME)

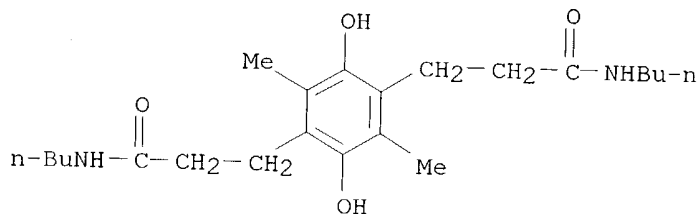


- L58 ANSWER 38 OF 47 HCA COPYRIGHT 2004 ACS on STN
 86:89291 Derivatives of arylalkylamines. VII. Some N-(arylalkyl)-substituted 3-phenyl-3-(hydroxyphenyl)propylamines. Markaryan, E. A.; Balayan, R. S. (Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR). Armyanskii Khimicheskii Zhurnal, 29(8), 704-7 (Russian) 1976. CODEN: AYKZAN. ISSN: 0515-9628. OTHER SOURCES: CASREACT 86:89291.
- AB Alkylation of C₆H₆ with 4-HOC₆H₄CH:CHCO₂Me afforded 50% 4-HOC₆H₄CHPhCH₂COX (I; X = OMe), which was saponified to give 76.3% I (X = OH) (II); treating II and its 2-hydroxy isomer with SOCl₂ and then RNH₂ [R = (MeO)₂C₆H₃CH₂CH₂, Ph₂CHCH₂CH₂, Ph₂CHCH₂CHMe, PhCH₂CH₂CHMe] afforded 70.3-96.3% yields of 7 corresponding I (X = NHR), which were reduced with LiAlH₄ to give 40.4-50.6% 2- and 4-HOC₆H₄CHPhCH₂CH₂NHR.
- IT **61904-47-0P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydride reduction of)
- RN 61904-47-0 HCA
- CN Benzenepropanamide, 2-hydroxy-N-(1-methyl-3,3-diphenylpropyl)- β -phenyl- (9CI) (CA INDEX NAME)

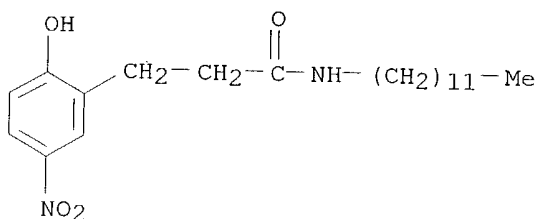


- L58 ANSWER 39 OF 47 HCA COPYRIGHT 2004 ACS on STN
 76:100115 Preparation and ring-opening polymerization of 2,5-

- dimethylhydroquinonebis-(8-lactone). Iwabuchi, Susumu; Ueda, Mitsuru; Kojima, Kuniharu (Fac. Eng., Chiba Univ., Chiba, Japan). Journal of Polymer Science, Polymer Chemistry Edition, 9(11), 3405-9 (English) 1971. CODEN: JPLCAT. ISSN: 0449-296X.
- AB 5,10-Dimethyl-3H,4H,8H,9H-benzo[1,2-b:4,5-b']dipyran-2,7-dione (I) [34375-11-6], the bislactone of 2,5-dimethylhydroquinone-3,6-bis(ethyl-2'-carboxylic acid), was prepared in 1 step by heating 1,4-dimethoxy-2,5-dimethyl-3,6-bis(2,2-dicarbethoxyethyl)benzene in HBr at 140-160.deg. for several hr. I was polymerized under N at 50-70.deg. in MeCONMe2 with diamines including hexamethylenediamine, m-xylylenediamine and piperazine. The polymers (II) were obtained in good yield in the form of white to light brown flakes. Uv spectra indicated that the II were obtained in the oxidized form (III).
- IT **35396-15-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 35396-15-7 HCA
- CN 1,4-Benzenedipropanamide, N,N'-dibutyl-2,5-dihydroxy-3,6-dimethyl- (9CI)
 (CA INDEX NAME)



- L58 ANSWER 40 OF 47 HCA COPYRIGHT 2004 ACS on STN
- 76:59248 Reducing agents for photographic processes. Bloom, Stanley M.; Huyffer, Paul S. (Polaroid Corp.). U.S. US 3622603 19711123, 7 pp. Division of U.S. 3,482,971 (CA 72;127282k). (English). CODEN: USXXAM. APPLICATION: US 1968-810047 19680916.
- GI For diagram(s), see printed CA Issue.
- AB Compds. useful as photographic reducing agents were prepared Thus, 6-nitrode-hydrocoumarin and n-C12H25NH2 heated in Me Cellosolve to dissoln. gave 2,5-HO(O2N)C6H3CH2CH2CONHC12H25-n. This, Me2SO4, and K2CO3 refluxed overnight in xylene gave the Me ether, which was hydrogenated in EtOH over Raney Ni to give 2,5-MeO(H2N)C6H3CH2CH2CONHC12H25-n. This, o-FC6H4-NO2, MgO, and H2O heated in a bomb 18 hr at 180° gave 2,5-MeO(o-O2NC6H4NH)C6H3CH2CH2CONHC12H25-n. The NO2 group was reduced to an NH2 group by hydrogenation over Pd/-BaSO4, the NH2 group acylated with p-O2NC6H4SO2Cl, and the product treated with BBr3 in CH2Cl2 to give I. Also prepared was II. Examples of use were given.
- IT **24355-41-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 24355-41-7 HCA
- CN Benzenepropanamide, N-dodecyl-2-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



L58 ANSWER 41 OF 47 HCA COPYRIGHT 2004 ACS on STN

72:91478 Dye developing 1-amino-2-[ω-[ω-(2,5-dihydroxyphenyl)alkanoylamino]alkylamino]-4-hydroxyanthraquinones. Downey, John F.; Simon, Myron S. (Polaroid Corp.). U.S. US 3491127 19700120, 7 pp. Division of U.S. 3347672 (English). CODEN: USXXAM. APPLICATION: US 1967-655582 19670724.

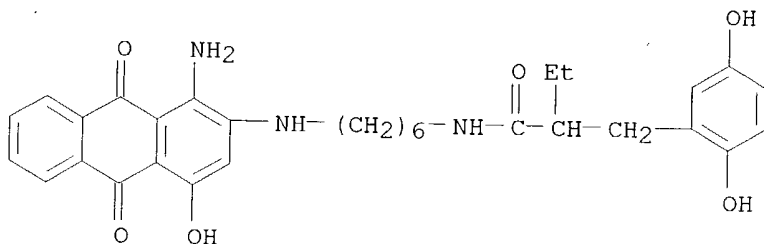
AB The disclosure is the same, but the claims are different.

IT **16618-31-8P**

RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)

RN 16618-31-8 HCA

CN Hydrocinnamamide, N-[6-[(1-amino-4-hydroxy-2-anthraquinonyl)amino]hexyl]-α-ethyl-2,5-dihydroxy- (8CI) (CA INDEX NAME)



L58 ANSWER 42 OF 47 HCA COPYRIGHT 2004 ACS on STN

72:3224 Scavengers for oxidized developing agent. Bloom, Stanley M.; Huyffer, Paul S. (Polaroid Corp.). U.S. US 3459548 19690805, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 1967-655309 19670724.

GI For diagram(s), see printed CA Issue.

AB A photographic element containing a light-sensitive Ag halide emulsion and a layer of a nondiffusible compound containing a color-providing moiety is exposed

and developed with an aqueous alkaline processing composition including a Ag halide

developing agent, and a scavenger for reducing oxidized developing agent formed to prevent a redox reaction with the nondiffusible compound. The reducing agents have the general structure I, (A is an anchoring substituent rendering the compound nondiffusible, B is a carboxy, alkoxy, alkyl, chloro, or an amide substituent, Q is an alkylene group, n is a pos. integer 1-3, m is 1-2 provided that where the alkylene moiety or together with B provides an anchoring substituent m may be 1, otherwise m must be 2). Thus, 38.6 g. 6-nitrodehydrocoumarin is dissolved in 400 ml. Me cellosolve, 28.4 g. n-octylamine added and the mixture heated on a steam bath 30 min. and cooled. Filtration yields 40.2 g. of a light yellow

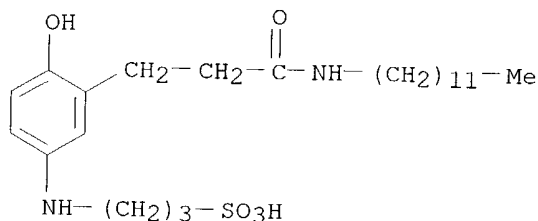
2,5-(HO)(O₂N)C₆H₃CH₂C H₂CONHC₈H₁₇, m. 179-80°, which, with 15.8 g. of propane sultone, 200 ml. of MeOH, and 5% Pd/BaSO₄, is placed in a pressure vessel. H is introduced and the reaction mixture shaken 4 hrs., 100 ml. MeOH added and the mixture boiled and filtered to give 23 g. 3,4-(C₈H₁₇NHCOCH₂-CH₂)(HO)C₆H₃N+H₂(CH₂)₃SO₃-, m. 196-7°. Similarly prepared were 2,5-(HO)(O₂N)C₆H₃CH₂CH₂CONHC₁₂H₂₅, m. 168-70°, and 3,4-(C₁₂H₂₅NHCOCH₂CH₂)(HO)C₆H₃N+H₂(CH₂)₃SO₃-, m. 207-8°.

IT **26601-03-6**

RL: RCT (Reactant); RACT (Reactant or reagent)
(as reducing agent in photographic processing)

RN 26601-03-6 HCA

CN 1-Propanesulfonic acid, 3-[3-[2-(dodecylcarbamoyl)ethyl]-4-hydroxyanilino]-(8CI) (CA INDEX NAME)



L58 ANSWER 43 OF 47 HCA COPYRIGHT 2004 ACS on STN

71:39538 Electron-transfer polymers. XL. Redox polyamides. Nakabayashi, Nobuo; Cassidy, Harold G. (Yale Univ., New Haven, CT, USA). Journal of Polymer Science, Polymer Chemistry Edition, 7(5), 1275-8 (English) 1969. CODEN: JPLCAT. ISSN: 0449-296X.

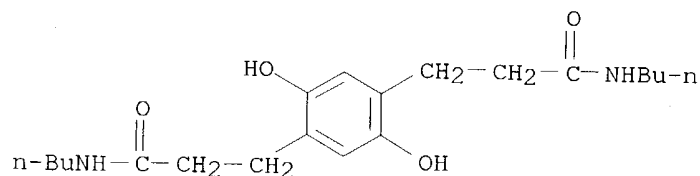
AB By condensing a hydroquinone bislactone of 2,5-bis(2-carboxyethyl)-1,4-dihydroxybenzene with diamines such as hexamethylenediamine, piperazine, 4-aminoethylpiperidine, or 1,3-di(4-piperidinyl)propane, redox polyamides can be prepared. The lactone functions protect the hydroxyl groups until the polymerization occurs, at which point, due to the opening of the lactone rings, free hydroquinone hydroxyls appear. The resulting polymer is oxidizable. When the oxidized polymer is reduced, the viscosity is higher than that of the original reduced polymer.

IT **24681-93-4**

RL: USES (Uses)
(model compds., for hydroquinone-based bislactone polyamide electron exchangers)

RN 24681-93-4 HCA

CN p-Benzenedipropionamide, N,N'-dibutyl-2,5-dihydroxy- (8CI) (CA INDEX NAME)



L58 ANSWER 44 OF 47 HCA COPYRIGHT 2004 ACS on STN

68:14102 1-Amino-2-[ω-(2,5-dihydroxyphenylacylamino)alkyl-amino]-4-hydroxyanthraquinone dye developers. Downey, John F.; Simon, Myron S. (Polaroid Corp.). U.S. US 3347672 19671017, 9 pp. (English). CODEN: USXXAM. APPLICATION: US 19631219.

GI For diagram(s), see printed CA Issue.

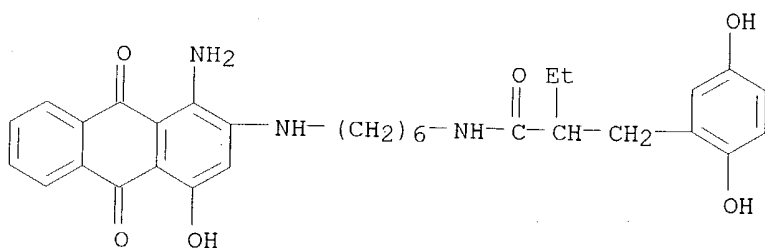
AB Compds. of the general formula I are prepared Thus, a mixture of 10 g. 1-amino-2-phenoxy-4-hydroxyanthraquinone and 100 ml. $\text{H}_2\text{N}(\text{CH}_2)_6\text{NH}_2$ is heated 3 hrs. to give 4.9 g. 1-amino-2-(6-aminoethylamino)-4-hydroxyanthraquinone (II), m. 193-6° (MeOH). Similarly prepared is 1-amino-2-(3-aminopropylamino)-4-hydroxyanthraquinone, m. 211-13° (MeOH). A mixture of 13.3 g. II, 7.5 g. 2,5-(HO)2C6H3CH2CH(Et)CO2H lactone, and 1020 ml. PhMe is heated 20 hrs. on a steam bath to give 15.9 g. I (m = 6, m = 1, R = Et) (III), m. 209-12° λ_{max} (MeOCH2CH2OH) 528, 565 nm. (ϵ = 20,600, 20,000). Similarly prepared are the following I [n, R, m, m.p., and λ_{max} (MeOCH2CH2OH) in nm. (ϵ + 10-4) given): 3, Et, 1, 225-8°, 529 (2.18) and 567 (2.08); 3, Me, 1, 225-8°, 529 (2.18) and 567 (2.08); 3, H, O, 187-99°, 527, 565; 6, Me, 1, 140-64°, 529, 565; 6, H, 1, 134-42°, 527, 565; 6, H, O, 134-42°, -, -. A gelatin film is coated with a solution of 0.15 g. III in 5 ml. 2% cellulose acetate hydrogen phthalate (in 50:50 Me2CO-tetrahydrofuran), a green-sensitive Ag(I, Br) emulsion is applied on the III layer to give a photosensitive element, and the element is exposed for 2 sec. A composition containing 100.00 ml. water, 11.20 g. KOH, 0.50 g. $\text{Zn}(\text{NO}_3)_2$, 4.00 g. Natrosol 250 (hydroxyethyl cellulose), 3.50 g. benzotriazole, 0.50 g. $\text{Na}_2\text{S}_2\text{O}_3$, and 2.00 g. N-benzyl- α -picolinium bromide is spread between the element and a superimposed receiver [baryta coated with 2:1 poly(vinyl alc.)-poly(4-vinylpyridine)], poly(vinyl alc.), and a half-Bu ester of poly(ethylene-maleic anhydride)]; a magenta-positive transfer image is obtained after an inhibition period of .apprx.1 min.

IT 16618-31-8P

RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)

RN 16618-31-8 HCA

CN Hydrocinnamamide, N-[6-[(1-amino-4-hydroxy-2-anthraquinonyl)amino]hexyl]- α -ethyl-2,5-dihydroxy- (8CI) (CA INDEX NAME)



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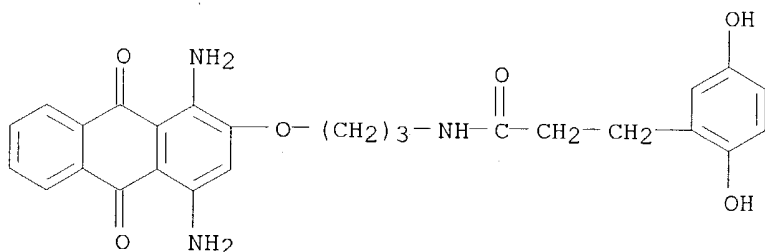
65:4441 Original Reference No. 65:844b-d Improved diazotype photoprinting process. (Copper Co., Ltd.). GB 1024489 19660330, 3 pp. (Unavailable). PRIORITY: JP 19630323.

GI For diagram(s), see printed CA Issue.

AB Compds. of formula I, where R and R1 are alkyl, hydroxyalkyl, aralkyl, or complete a morpholine or piperidine ring, have improved solubility and coupling properties when used in 1- and 2-component diazo processes. A solution of 2,4-Br(MeO)C6H3OH, m. 45°, and KOH was treated with BuBr to give

3,4-Br(BuO)C₆H₃OMe (II), b₅ 125°. II nitrated in AcOH gave 4,2,5-Br(MeO)(BuO)C₆H₂NO₂ (III), m. 68°. III refluxed in morpholine gave 4,2,5-Q(MeO)(BuO)C₆H₂NO₂ (Q = morpholino), m. 85°, which was reduced and diazotized to give the corresponding I (IV). Paper was coated with a solution of IV 20, citric acid 3, and thiourea 10 g. in 1000 cc. of H₂O, exposed, and developed with a solution of borax 15, K₂CO₃ 15, and 2,3,6-HOC₁₀H₅(SO₃H)₂ (V) 15 g. in 1000 cc. of H₂O to give a violet print. Similarly used were I (R + R₁ + N = piperidino) and I (R = Me, R₁ = CH₂CH₂OH), the latter in a 2-component process with V as coupler and NH₃ as developer.

- IT **6398-88-5**, Hydrocinnamamide, N-[3-[(1,4-diamino-2-anthraquinonyl)oxy]propyl]-2,5-dihydroxy-
(manufacture and use as photographic developer)
RN 6398-88-5 HCA
CN Benzenepropanamide, N-[3-[(1,4-diamino-9,10-dihydro-9,10-dioxo-2-anthracenyl)oxy]propyl]-2,5-dihydroxy- (9CI) (CA INDEX NAME)



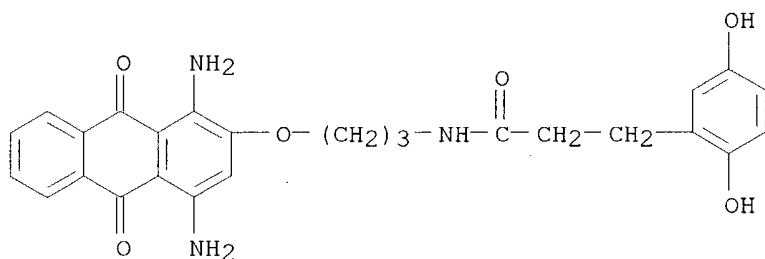
L58 ANSWER 46 OF 47 HCA COPYRIGHT 2004 ACS on STN

65:4439 Original Reference No. 65:843g-h,844a Dye developer. Downey, John F.; Simon, Myron S. (Polaroid Corp.). US 3245790 19660412, 5 pp. (Unavailable). APPLICATION: US 19611113.

GI For diagram(s), see printed CA Issue.

AB cf. following abstract Novel photographic processes are presented which employ anthraquinone compds. (I) having the ability to develop images present in an exposed Ag halide emulsion. I are prepared by treating a 1,4-di-amino-g-(w-aminoalkoxy)anthraquinone with the lactone II of 2,5-(HO)₂C₆H₄CH₂CH₂CO₂H in EtOH under N. Thus, a mixture of 34.9 g. 1,4-diamino-2-(e-aminoamyloxy)anthraquinone, 29.4 g. II and 350 cc. EtOH is deaerated with N and heated for 16 hrs. on a steam-bath, cooled to 25°, and diluted with 13.5 g. NaOH in deaerated H₂O. After 0.5 hr., CO₂ is bubbled in until the pH remains constant, the mixture is filtered, the residue is washed to a colorless filtrate with 3% HCl, and then with H₂O until the cake is acid-free, to give I (n = 4, R = H), m. 157-8° (iso-PrOH), λ_{maximum} 577 mμ (ε 16,000). Similarly prepared are the following I (n, R, and m.p. given): 1, H, 174-84°; 2, H, 141-4°; 1, Et, 124-34°. Typical formulations and processes are given.

- IT **6398-88-5**, Hydrocinnamamide, N-[3-[(1,4-diamino-2-anthraquinonyl)oxy]propyl]-2,5-dihydroxy-
(manufacture and use as photographic developer)
RN 6398-88-5 HCA
CN Benzenepropanamide, N-[3-[(1,4-diamino-9,10-dihydro-9,10-dioxo-2-anthracenyl)oxy]propyl]-2,5-dihydroxy- (9CI) (CA INDEX NAME)



L58 ANSWER 47 OF 47 HCA COPYRIGHT 2004 ACS on STN

61:69041 Original Reference No. 61:11961a-c Pyran series; its analogs and related compounds. IX. Reaction of coumarin with amines. Zagorevskii, V. A.; Savel'ev., V. L. Zhurnal Obshchei Khimii, 34(7), 2290-3 (Unavailable) 1964. CODEN: ZOKHA4. ISSN: 0044-460X.

GI For diagram(s), see printed CA Issue.

AB Heating 5 g. coumarin with 15 g. piperidine in EtOH 2 hrs. at 60°, then keeping 16 hrs. at room temperature gave 79% β-piperidino-o-hydroxyhydrocinnamopiperidide (I), m. 85-6°, isolated from aqueous HCl extract, and a small amount o-hydroxycinnamopiperidide (II), m. 221-2° (decomposition), from the organic layer. The yields were 74% and 17% in 2 hrs. at

110° and 48 hrs. at room temperature I and piperidine heated at 110° 2 hrs. and kept 2 days gave II in 17% yield. Similarly, II was converted into 17% I. Heating I with concentrated HCl 6 hrs. gave coumarin.

Coumarin refluxed 17 hrs. with Et₂NH gave 16% β-diethylamino-o-hydroxyhydrocinnamoN,N-diethylamide, isolated as the HCl salt, m. 145-6°, and 1.3% o-hydroxycinnamo-N,N-diethylamide, m.

168-70°, hydrogenated over Pd to the hydrocinnamic analog, m. 129-30°. Coumarin and BuNH₂ in 12 hrs. gave 46%

β-butylamino-o-hydroxyhydrocinnamo-N-butylamide, isolated as the HCl salt, m. 134-6°, and 2% o-hydroxycinnamo-N-butylamide, m.

157-8°. Cyclohexylamine in 12 hrs. at 100° gave 8% o-hydroxycinnamoN-cyclohexylamide, decomposed 223-4°, and 92%

β-cyclohexyl- amino-o-hydroxyhydrocinnamo-N-cyclohexylamide, m.

124-5° (decomposition). Coumarin and benzylamine in 12 hrs. similarly gave 5.6% o-hydroxycinnamo-N-benzylamide, decomposed 180.51.5°, and

some 80% β-benzylamino-o-hydroxyhydrocinnamoN-benzylamide,

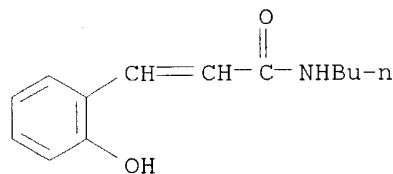
decompd. 97.4-99°. Bu₂NH in 12 hrs. at 160° similarly gave 62% unreacted coumarin and 18% o-hydroxy- cinnamo-N,N-dibutylamide, m.

96.5-7.5°; in 15 hrs. at 100° 86% coumarin was recovered.

IT 92040-78-3, Cinnamamide, N-butyl-o-hydroxy- (preparation of)

RN 92040-78-3 HCA

CN Cinnamamide, N-butyl-o-hydroxy- (7CI) (CA INDEX NAME)



Hardee

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08/18/2004

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